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FLUID MECHANICS AND TRANSPORT PHENOMENA

An Analogy between Reaction and Heat Transfer

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A relationship between the Nusselt number and the chemical conversion arising from an energetic reaction in fully developed laminar or turbulent flow through a heated or cooled tube is formulated by the speculative adaptation and extension of a closed-form solution for an idealized case. This relationship may be interpreted as an analogy between reaction and heat transfer. It has a wider scope than the classical analogies between momentum and heat transfer but is inferior to them in the sense that it incorporates an arbitrary coefficient whose dependencies have not yet been completely resolved. The analogy was derived for a single first-order irreversible equimolar homogeneous reaction (restrictions that can be relaxed) and neglects entrance effects and changes in density and viscosity. The primary and unique contribution of the analogy is the mathematical representation and functional explanation of the chaotic and gross variation of the Nusselt number resulting from the combination of an energetic reaction and compensatory heat exchange. © 2006 American Institute of Chemical Engineers *AIChE J,* 52: 3645–3657, 2006
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Introduction

When gas-phase chemical reactions are carried out in steady flow through a tube, heating at the outer surface may be necessary to initiate the reaction. If the reactions are endothermic, heating may also be required to prevent premature self-quenching because of the resulting decrease in temperature. If the reactions are exothermic, cooling may be necessary to minimize undesirable side reactions associated with an excessive temperature and/or to prevent a thermal runaway.

A number of prior theoretical analyses and experimental investigations have revealed that energetic reactions may greatly enhance or mildly attenuate the rate of compensatory heat exchange as characterized by the Nusselt number. Unfortunately, these prior investigations of combined reaction and convection are fragmentary and incoherent, and have generally been overlooked in the literature of both heat transfer and reaction engineering. One objective of the long-term investigation—of which the current work is a part— is to evaluate such enhancements and attenuations systematically and quantitatively by means of the numerical solution of the differential equations of conservation and, insofar as possible, to explain the results qualitatively and devise generalized predictive or correlative expressions for the behavior.

The objective of the phase of the work reported here is limited to the development of an analogy between the fractional conversion arising from an energetic chemical reaction and the Nusselt number for compensatory heat exchange when they occur simultaneously. The expectation is that such an analogy will prove useful in explaining, if not predicting, the interactions between reaction and heat transfer just as have the classical analogies for momentum transfer and heat transfer. The development of an analogy that encompasses the aforementioned enhancements and attenuations would appear to be a worthy objective but a formidable challenge.

Two thermal boundary conditions are considered: (1) a uniform heat flux density through the wall of the tube and (2) a uniform wall temperature. A uniform heat flux density has been the thermal boundary condition of choice in most theoretical analyses of forced convection with and without an energetic chemical reaction because the mathematical formulations and processes of solution are then the simplest. Such a condition can be closely approximated in practice by countercurrent heat exchange between fluid streams in the inner and outer passages of an annulus. Herein, the reacting fluid is postulated to flow through the inner tube. In the case of heating but not cooling, a uniform heat flux density may also be attained with a single tube by means of electrical-resistance heating of the wall. On

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the other hand, a uniform temperature can be imposed to a good approximation by means of an external condensing fluid for cooling or an external boiling fluid for heating.

The modeling of energetic chemical conversions is much more difficult than the modeling of pure convection because of the involvement of multiple reaction mechanisms in most chemical processes, each of which depends exponentially and differently on temperature and many of which are nonequimolar. The general model for combined reaction and heat transfer consists of a set of partial differential equations (PDEs) for the conservation of species that are nonlinear in temperature, generally nonlinear in concentration, and strongly coupled with the PDE for the conservation of energy as well as with each other. The number of significant rate mechanisms, independent chemical species, and parameters associated with the rate mechanisms may exceed 100, 20, and 50, respectively. This multiplicity is to be contrasted with pure convection, which, insofar as the flow is fully developed and variation of the physical properties with temperature is neglected, may be modeled by a single linear PDE, a single dependent variable (temperature), and three parameters (the Reynolds number, the Prandtl number, and the mode of heat transfer at the wall). Herein, in the interests of simplicity and insight, and as a first step, only a single, first-order, irreversible, equimolar but temperature-dependent reaction-rate mechanism is considered.

Analogies for Momentum and Heat Transfer in Turbulent Flow

Analogies between momentum and heat transfer provide better predictive and correlative expressions for convective heat transfer in turbulent tubular flow than do purely empirical ones. The best-known analogies are those of Reynolds,[1] Prandtl,[2] and Colburn,[3] but that of Reichardt[4] is their superior. A brief review of the derivation and limitations of these four analogies provides a background for the development of perhaps the first-ever analogy between chemical reaction and heat transfer but is hardly a template, given that a chemical reaction is not in itself analogous to transport.

Reynolds in 1874 derived an analogy that can be expressed as follows:

$$\mathrm{Nu} = \mathrm{PrRe}(f/2) \tag{1}$$

The critical element in the derivation of Eq. 1 is the postulate that momentum and energy are carried at equal rates from the bulk of the fluid to the wall by the oscillatory motion of eddies. That postulate avoids the need for a mechanistic model and any arbitrary coefficients. Subsequent analyses have revealed that Eq. 1 is valid functionally only for $\mathrm{Pr} = \mathrm{Pr}_t \cong 0.86$ and is in significant numerical error for other values of Pr. However, Eq. 1 has proven to be of lasting value as a prototype, and it appears to this day as a component of many more complex expressions for turbulent convection.

Prandtl in 1910 improved on the Reynolds analogy by postulating that the turbulent eddies penetrate only to a finite distance δ from the wall, and that transport of momentum and energy through that *boundary layer* occurs by linear diffusion. His analogy can be expressed as

$$\mathrm{Nu} = \frac{\mathrm{PrRe}f/2}{1 + \delta^+(\mathrm{Pr} - 1)(f/2)^{1/2}} \tag{2}$$

The Prandtl analogy was an influential step forward in that it correctly predicted an interlinked dependency of Nu on Pr and Re. However, the Prandtl analogy shares the shortcoming of the Reynolds analogy for $\mathrm{Pr} = \mathrm{Pr}_t \cong 0.861$, fails outright for $\mathrm{Pr} < 1$, and, because of its failure to account for turbulent transport within the viscous boundary layer, predicts the wrong dependencies on Pr and Re for $\mathrm{Pr} \to \infty$. The dimensionless boundary layer thickness δ^+ depends on Re, and Jakob[5] referring to the equivalent of δ^+, noted that "There exists a whole literature about this ratio."

Colburn in 1933 observed that an empirical expression for Nu and another one for $f/2$ had nearly the same leading coefficient, suggesting to him that these coefficients could be eliminated (to a fair degree of approximation) by taking the ratio of the two expressions. Exponents of 0.3 and 0.4 for Pr, for cooling and heating of the fluid, respectively, were replaced "for convenience" by 1/3, resulting in

$$\mathrm{Nu} = \mathrm{Pr}^{1/3}\mathrm{Re}^{0.8}f/2 \tag{3}$$

The Colburn analogy is in error functionally in almost every respect and thereby can be considered a step backward from the Prandtl analogy in a theoretical sense. However, in spite of its functional shortcomings, and indeed because of its empirical origin, Eq. 3 provides numerical predictions of moderate accuracy and it remains in service today in some computer packages for process design.

Reichardt in 1950 derived a substantially improved analogy in a theoretical sense. He combined the two-dimensional differential momentum and energy balances to obtain a single ordinary differential equation in terms of the radius, and introduced an algebraic expression for turbulent transport in the boundary layer. Then, to permit integration of the resulting expression in closed form, he made some ingenious mathematical approximations that are applicable for large and moderate values of Pr. These approximations imply a uniform wall temperature. Improvements and adaptations have since been made by a number of investigators (see Churchill[6] for a discussion thereof). As an example of such modifications, Churchill and Zajic[7] not only improved on the Reichardt analogy by substituting a more accurate expression, both functionally and numerically, for the contribution of the turbulent fluctuations, but also generalized this analogy for uniform heating as well as uniform wall temperature. Their final result can be expressed as follows:

$$\mathrm{Nu} = \left[\frac{2\gamma}{\mathrm{Re}f}\left(\frac{\mathrm{Pr}_t}{\mathrm{Pr}}\right) + \frac{13.62}{\mathrm{Re}(f/2)^{1/2}}\left(\left[\frac{\mathrm{Pr}_t}{\mathrm{Pr}}\right]^{1/3} - 1\right)\right]^{-1} \tag{4}$$

Here, γ is a theoretically defined integral that depends mildly on Re, $\mathrm{Pr}_t/\mathrm{Pr}$, and the thermal boundary condition at the wall.

All of the analogies mentioned above, including Eq. 4, are limited in applicability to large and moderate values of Pr, but Churchill and Zajic also devised a complementary expression for $\mathrm{Pr} \leq \mathrm{Pr}_t \cong 0.86$, which need not be reproduced here.

The purpose of this digression is to serve as a guide and

Table 1. Coefficient β for Fully Developed Turbulent Convection with Volumetrically Uniform Heating as a Function of Re and Pr

		Pr						
a^+	Re	0.01	0.10	0.70	0.8673	1.0	10	100
500	17,000	0.0992	0.0782	0.0491	0.0461	0.0441	0.0203	0.00912
1000	37,640	0.0843	0.0609	0.0360	0.0335	0.0319	0.0132	0.00532
5000	227,000	0.0606	0.0371	0.0212	0.0197	0.0187	0.00663	0.00204
10,000	486,000	0.0521	0.0308	0.0179	0.0166	0.0158	0.00551	0.00156

point of referral for the derivations that follow for the combination of an energetic chemical reaction and heat exchange. The most important inference to be drawn from the above analogies between momentum and heat transfer is that they have resulted in theoretical structures that might not otherwise have been deduced. A second inference is that the process of deriving an analogy is not necessarily straightforward and may require insight, imagination, and persistence. A third inference is that the idealizations and constraints are often implicit and not easy to identify.

To avoid excessive expectations for an analogy between reaction and heat transfer, it should be noted that implementation of any of the above analogies to predict heat transfer requires a supplemental expression to predict the friction factor. Also, it should be noted that the Prandtl analogy incorporates an unspecified function (δ^+), that the Colburn analogy incorporates an implicit empirical coefficient (of unity) and two explicit empirical exponents (0.8 and 1/3), that the Churchill–Zajic modification of the Reichardt analogy incorporates an empirical coefficient (13.62) arising from the representation of the turbulent transport near the wall, and a theoretically based function, that is, $\gamma\{\text{Re, Pr, mode}\}$. Furthermore, an energetic chemical reaction invokes many variables and dependencies in addition to those for pure convection.

The Crucial Step in Devising an Analogy between Reaction and Heat Transfer

The step that proved absolutely crucial to what follows was the prior derivation by Churchill[8] of an exact solution in closed form for a very idealized process of flow, reaction, and heat transfer—that is, fully developed convection in fully developed laminar flow through a round tube with a volumetrically uniform rate of reaction, a uniform heat flux density through the wall, and radial conduction of heat, but no radial diffusion of species. A volumetrically uniform rate of reaction might be rationalized on the basis of asymptotically small perturbations in the composition attributed to the reaction and in the temperature attributed to the combination of the heat of reaction and the imposed heat flux. In any event, the solution can be expressed as

$$\text{Nu} = \frac{48/11}{1 + 3Q/11} \tag{5}$$

Here, Q represents the dimensionless ratio of the volumetrically uniform input of energy by reaction to the uniform heat flux density from the wall. As $Q \to 0$, Nu $\to 48/11$, which is the well-known solution for fully developed laminar convection with uniform heating or cooling and no reaction. For negative values of Q, corresponding to the combination of an endothermic reaction and heating through the wall or to an exothermic reaction and cooling through the wall, Nu increases and becomes unbounded as $-3Q/11$ increases in magnitude and approaches unity. For the thermally unbalanced case of a positive value of Q, corresponding to an exothermic reaction and heating from the wall, or the converse of both, Nu is seen from Eq. 5 to decrease slowly as Q increases. Equation 5 has exactly the same form as the well-known solution for the effect of viscous dissipation on the heat-transfer coefficient. Despite the gross idealizations, the predicted effects of Eq. 5 for positive and negative values of Q are given credence by their qualitative congruence with prior theoretical and experimental predictions of enhancement and attenuation arising from energetic reactions. Most important, Eq. 5 can be interpreted as an analogy between the rates of chemical reaction and of heat transfer, as represented by Q and Nu/(48/11), respectively, with a theoretical coefficient of 3/11.

A solution in closed form for turbulent flow is not feasible even for the extremely idealized conditions that led to Eq. 5 for laminar flow. However, it may be speculated that the form of Eq. 5 with an empirical coefficient β in place of 3/11 and an appropriate asymptotic value in place of 48/11 might prove useful as a correlative expression and/or an analogy. Such an expression is

$$\text{Nu} = \frac{\text{Nu}_o}{1 + \beta Q} \tag{6}$$

Here, Nu_o is the Nusselt number for fully developed turbulent convection with no heat of reaction. In the context of an analogy, the dimensionless rates of chemical reaction and convection are now represented by Q and Nu/Nu_o, respectively. As may be inferred from Eq. 6, enhancement and attenuation of Nu are characterized by the product βQ.

Equation 6 was tested with essentially exact numerically calculated values of Nu for turbulent flow for a wide range of values of Re, Pr, and Q, but otherwise the same conditions as those for which Eq. 5 was derived. The corresponding values of β, listed in Table 1, not only differ from the fixed value for laminar flow, but also display a moderate and monotonic dependency on Re and Pr. This dependency is disappointing, but that disappointment is assuaged by the complete independence, as is illustrated in Table 2 for Pr = 0.7 and four values of the Reynolds number, of β from the parameter Q. Because the small variance in the values of β for a given value of Re can safely be assigned to numerical error and extreme sensitivity, the invariance must have an inherent theoretical basis. That particular invariance encouraged the development that follows.

Table 2. Coefficient β for Fully Developed Turbulent Convection at Pr = 0.70 as a Function of the Rate of Volumetrically Uniform Heating

Q	$\frac{a^+}{\mathrm{Re}}$	$\frac{500}{17{,}000}$	$\frac{1000}{37{,}640}$	$\frac{5000}{226{,}900}$	$\frac{10{,}000}{485{,}900}$
0.10		0.05000	0.03514	0.02158	0.01732
0.50		0.04892	0.03587	0.02122	0.01773
1.00		0.04900	0.03692	0.02117	0.01789
5.00		0.04907	0.03595	0.02126	0.01794
10.00		0.04909	0.03585	0.02125	0.01793
20.00		0.04907	0.03595	0.02122	0.01792
100.00		0.04908	0.03597	0.02122	0.01793

Adaptation of the Analogy for Developing Reaction and Convection

Equations 5 and 6 are actually simpler than any of the classical analogies for momentum and heat transfer, but that is not the case for what follows. On purely speculative grounds and without great expectations, Eq. 6 was rewritten as follows for the much more complex and realistic case of developing reaction and developing convection:

$$\mathrm{Nu}_x = \frac{\mathrm{Nu}_{ox}}{1 + \beta Q_x} \tag{7}$$

Here the subscript x designates a quantity varying with axial length and, as before, the subscript o designates a value in the absence of reaction. The quantity Q_x is the dimensionless rate of reaction at x, the corresponding dimensionless rate of convection is $\mathrm{Nu}_x/\mathrm{Nu}_{ox}$, and β is again an empirical coefficient.

For uniform heating or cooling at the wall (Q_x), the ratio of the input of energy by reaction to the heat flux from the wall in a differential length of the reactor, may be expressed as follows:

$$Q_x = \frac{\pi a^2 C_{A0}(1 - Z_{mx}) k q_M}{2\pi a j_w} = \frac{\tau\, \mathrm{RePr} K_{a0}(1 - Z_{mx})}{4J} = \xi(1 - Z_{mx}) \tag{8}$$

Here, Z is the fractional chemical conversion of species A; k is the reaction-rate constant; a subscript 0, not to be confused with a subscript o, designates a value at the entrance; a subscript m designates a mixed-mean value, that is, the integrated mean with respect to radius, weighted by the time-averaged velocity distribution; $K_{a0} \equiv k_0 a/u_m$ is the dimensionless rate of reaction; $\tau \equiv q_M/c_M T_0$ is the *thermicity*, that is, the increase in temperature resulting from an exothermic reaction ($q_M > 0$) or the decrease resulting from an endothermic reaction ($q_M < 0$); T_0 is the absolute temperature at the entrance; and $J \equiv a j_w/\lambda T_0$ is the dimensionless heat flux density from the wall to the fluid. The quantity J is an obvious analogue of Nu, but for uniform heating it is a specified parameter rather than a dependent variable. The factor $\xi \equiv \tau \mathrm{RePr} K_{a0}/4J$ is a combination of the specified variables in Eq. 8, that is, those that do not vary with the primary independent variable $K_{x0} \equiv k_0 x/u_m$, the dimensionless length of the zone of reaction. In practice, J and τ ordinarily have opposite signs, resulting in a negative value for ξ as well as for Q_x.

It is implied in the formulation of Eq. 8 and by the dimensionless groupings therein that the physical properties are independent of temperature and composition even though the latter two quantities ordinarily vary significantly with both radius and length within a tubular reactor. The resulting variation of the density and viscosity of the fluid may not be significant, but that of the reaction-rate constant is ordinarily too great to ignore. Therefore the following modification of Eq. 8 is proposed. First, the dependency of the reaction-rate constant on temperature is postulated to be given by the Arrhenius equation, that is,

$$k = k_\infty e^{-(E/RT)} = k_0 e^{E/RT_0[1-(T_0/T)]} \tag{9}$$

The right-most form of Eq. 9, which was apparently first introduced by Churchill,[8] is used exclusively herein. The quantity k_0 is the reaction-rate constant at the inlet temperature T_0, as contrasted with the more familiar quantity k_∞, the reaction-rate constant for an infinite temperature. Although Eq. 9, in either form, is empirical, it has a theoretical rationale and has generally been found to reproduce experimental data for any one reaction mechanism with sufficient accuracy for all practical purposes.

Next, to take the variation of the reaction-rate constant according to Eq. 9 into account in the reactor, the right-most form of Eq. 8 is reexpressed as

$$Q_x = \left(\frac{k_{emx}}{k_0}\right)\xi(1 - Z_{mx}) \tag{10}$$

Here k_{emx} is the effective-mean value of the rate constant over the cross section at x. With these supplementations, Eq. 7 can be reexpressed as

$$\mathrm{Nu}_x = \frac{\mathrm{Nu}_{xo}}{1 + \beta(k_{emx}/k_0)\xi(1 - Z_{mx})} \tag{11}$$

The following approximation is proposed for k_{emx}:

$$\frac{k_{emx}}{k_0} \cong \frac{k\{T_{mx}\}}{k\{T_0\}} = \frac{k_\infty e^{-E/RT_{mx}}}{k_\infty e^{-E/RT_0}} = e^{E/RT_0[1-(T_0/T_{mx})]} \tag{12}$$

Equation 12 is based on the speculation that the effective value of the rate constant does not differ significantly from its value at the mixed-mean temperature.

To implement Eq. 12 in the context of the analogy, an

expression is needed for the mixed-mean temperature ratio T_{mx}/T_0 in terms of the mixed-mean conversion Z_{mx}. The following exact energy balance over a length of the reactor from the entrance to any length x provides that relationship:

$$u_m \pi a^2 (T_{mx} - T_0) c\rho = C_{A0} Z_{mx} q_M u_m \pi a^2 x + 2\pi a x j_w \quad (13)$$

Equation 13 can be rearranged and reexpressed in the following forms:

$$\frac{T_{mx}}{T_0} = 1 + \frac{C_{A0} Z_{mx} q_M x}{\rho c u_m T_0} + \frac{2 j_w x}{a u_m \rho c T_0} = 1 + Z_{mx}\tau + \left(\frac{4K_{x0}}{\mathrm{RePr}K_{a0}}\right) J \quad (14)$$

The second and third terms on the right-hand side of Eq. 14 represent the contributions of reaction and heat exchange, respectively, to the mixed-mean temperature.

Equation 11 constitutes the basic analogy between reaction and heat transfer, but Eqs. 12 and 14 are needed for its implementation. These three equations can be combined to obtain the following expanded expression of the analogy in terms of Z_{mx}, and the parameters Nu_{ox}, K_{x0}, E/RT_0, τ, and ξ:

$$\mathrm{Nu}_x = \frac{\mathrm{Nu}_{ox}}{1 + \beta\xi(1 - Z_{mx})\exp\left\{\dfrac{E/RT_0}{1 + (\tau[Z_{mx} + (K_{x0}/\xi)])^{-1}}\right\}} \quad (15)$$

Equation 15, which provides a relationship between the local Nusselt number and the local mixed-mean conversion, incorporates a number of fixed parameters and one arbitrary coefficient, that is, β. That coefficient is the counterpart of the arbitrary coefficients, exponents, and exponents of Eqs. 2–4. Just as with Eqs. 1–4, Eq. 15 includes implicit idealizations in structure. In this case the implicit idealizations are those of Eqs. 7 and 12.

A discussion of the merits and shortcomings of this analogy for a uniform heat flux is deferred until after the derivation of its counterpart for a uniform wall temperature.

An Analogy for Uniform Wall Temperature

For uniform heating the three dependent variables—Nu_x, Z_{mx}, and T_{mx}/T_0—can be reduced to two by virtue of Eq. 14, thereby allowing the formulation of a direct relationship between Nu_x and Z_{mx}, that is, Eq. 15. For a uniform wall temperature, it does not appear possible to develop a simple theoretical relationship between two of the four dependent variables Nu_x, Z_{mx}, T_{mx}/T_0, and $J_x \equiv aj_w/\lambda T_0$. One alternative is the speculation that Eq. 11 remains valid if J_x is simply substituted for J, that is, if ξ is replaced by $\xi_x \equiv \tau\mathrm{RePr}K_{a0}/4J_x$. For a uniform wall temperature, the expanded form of the analogy is thus

$$\mathrm{Nu}_x = \frac{\mathrm{Nu}_{oxT}}{1 + \beta\xi_x(1 - Z_{mx})\exp\left\{\dfrac{E}{RT_0}\left(1 - \dfrac{T_0}{T_{mx}}\right)\right\}} \quad (16)$$

Here, Nu_{oxT} is the Nusselt number for pure forced convection with a uniform wall temperature.

The dependent variable J_x may be replaced by the alternative dependent variable T_{mx}/T_0 by virtue of the definition of the local Nusselt number, that is,

$$\mathrm{Nu}_x = \frac{2aj_w}{\lambda(T_w - T_m)} = \frac{2J_x}{\dfrac{T_w}{T_0} - \dfrac{T_{mx}}{T_0}} \quad (17)$$

It follows from Eq. 17 that

$$\xi_x = \frac{\tau\mathrm{RePr}K_{a0}}{2\,\mathrm{Nu}_x\left(\dfrac{T_w}{T_0} - \dfrac{T_{mx}}{T_0}\right)} \equiv \frac{\zeta}{\mathrm{Nu}_x\left(\dfrac{T_w}{T_0} - \dfrac{T_{mx}}{T_0}\right)} \quad (18)$$

Here $\zeta \equiv \tau\mathrm{RePr}K_{a0}/2$ is the characteristic group of specified variables for a uniform wall temperature. Then

$$\mathrm{Nu}_x = \frac{\mathrm{Nu}_{oxT}}{1 + \left(\dfrac{\beta\zeta(1 - Z_{mx})}{\mathrm{Nu}_x\left(\dfrac{T_w}{T_0} - \dfrac{T_{mx}}{T_0}\right)}\right)\exp\left\{\dfrac{E}{RT_0}\left(1 - \dfrac{T_0}{T_{mx}}\right)\right\}} \quad (19)$$

Equation 19 can be rearranged as follows to be explicit in terms of Nu_x:

$$\mathrm{Nu}_x = \mathrm{Nu}_{oxT} - \left(\frac{\beta\zeta(1 - Z_{mx})}{\dfrac{T_w}{T_0} - \dfrac{T_{mx}}{T_0}}\right)\exp\left\{\frac{E}{RT_0}\left(1 - \frac{T_0}{T_{mx}}\right)\right\} \quad (20)$$

It should be noted that a value of T_w is ordinarily chosen to be $<T_0$ and T_{mx} when τ is positive and vice versa.

Equations 16 and 20 both incorporate a dependent variable (either J_x, or ξ_x or T_{mx}/T_0) in addition to Z_{mx}, and in that respect suffer from comparison with Eq. 15. Even so, they have possible value in predicting the effect of the various parameters that are encompassed. Equation 20 has a small advantage over Eq. 16 in that the local mixed-mean temperature is more readily calculated than J_x.

Utilization, Evaluation, and Interpretation of the Analogies

The mixed-mean conversion (Z_{mx}) in the proposed analogy between developing chemical reaction and heat transfer is the counterpart of the friction factor (f), in the various analogies between fully developed momentum and heat transfer. The friction factor for fully developed flow in a smooth round tube is a function of the Reynolds number only. On the other hand, the mixed-mean conversion is a function of the dimensionless distance through the tube, the dimensionless rate of heat exchange with the wall, and all of the dimensionless variables and parameters that determine the rate of reaction. This complex dependency might appear to preclude the derivation of an algebraic expression for Z_{mx} as function of τ and J, but Churchill and Yu[9] devised a set of empirical expressions that can be consolidated to the following expression:

Table 3. Variance of Coefficient β with the Thermicity and Heat Flux Density Laminar Flow at Re = 400 and K_{x0} = 0.50, for Which Nu_{ox} = 6.2994, Pr = 0.7, Sc = 0.2, E/RT_0 = 17.815, and T_0 = 300 K

τ	J	$-\xi$	Z_m	Nu_x	T_{mx}/T_0	k_{lmx}/k_0	β
0.01	−0.10	0.672	0.35533	6.7047	0.99517	0.93342	0.14956
0.01	−0.05	1.344	0.37215	7.4208	1.00002	1.00033	0.17903
0.05	−0.10	3.36	0.40865	10.7279	1.01303	1.25745	0.16522
0.05	−0.05	6.72	0.43155	161.3508	1.01785	1.36732	0.18398
−0.01	0.10	0.672	0.40121	7.1183	1.03394	1.06211	0.26918
−0.01	0.05	1.344	0.32081	7.8202	0.99987	0.99777	0.23496
−0.05	0.10	3.36	0.35408	11.5157	0.98970	0.83080	0.25122
−0.05	0.05	6.72	0.33948	27.0054	0.98673	0.78694	0.21949

$$Z_{mx} = \frac{1 - e^{-0.96K_{0x}}}{1 - 3.85\tau} + \frac{250JK_{0x}}{\mathrm{Re}} \tag{21}$$

Equation 21 provides reasonable predictions for uniform heating for all conditions. Although Churchill and Yu[9] also devised an empirical expression for the prediction of Z_{mx} for uniform wall temperature, it is not reproduced here because Eqs. 16 and 20 are not proposed for quantitative predictions.

The coefficient β in the proposed analogy for chemical reaction and heat transfer is the counterpart of δ^+ in the analogy of Prandtl, γ in the Churchill–Zajic modification of the analogy of Reichardt, and the implicit numerical coefficient (chosen for convenience as unity) in the analogies of Reynolds and Colburn. As mentioned in connection with Eqs. 2 and 4, the quantity δ^+ is an as yet unresolved function of Re, Pr, and the mode of heat transfer at the wall, and the quantity γ is an integral of the velocity distribution for a uniform heat flux density and of the temperature distribution as well for a uniform wall temperature.

Ideally, β would have a single fixed value for all conditions, that is, for all values of K_{x0}, K_{a0}, Re, Pr, Sc, τ, E/RT_0, T_0, and J or T_w/T_0. The difference noted between the value of β for fully developed laminar convection and fully turbulent convection, and the dependency of β on Re and Pr in the latter regime, even for the super-idealized case of volumetrically uniform reaction and no diffusion, extinguished that hope, although the independence of β from Q was encouraging and led to the speculative formulation of Eq. 7 and its detailed implementation in terms of Eqs. 15, 16, and 20. The next best result would be a generalized and/or theoretically based expression for β analogous to that for γ.

As a first step in the attempt to devise such an expression, values of β were calculated from the values of Nu_x and Z_{mx} computed by Yu and Churchill,[10,11] who solved the PDEs of conservation by finite-difference methods for a uniform heat flux at the wall and a uniform wall temperature, respectively. Their tests of convergence with grid size and their comparisons with theoretical and prior numerical solutions for no reaction indicate that the finite-difference solutions are exact for all practical purposes. In the interests of clarity, the calculated values of β for laminar and turbulent flow, and for a uniform heat flux and a uniform wall temperature, are examined separately. Because the focus herein is on the analogy, the computed values of Z_{mx} by Yu and Churchill,[10,11] rather than those predicted by Eq. 21, were used to calculate β.

Laminar flow with uniform heating and cooling

The values of β for a uniform heat flux were determined from Eq. 15. The values of β thus computed at the arbitrary but representative value of K_{x0} = 0.50 are illustrated in Table 3 for the eight conditions chosen by Churchill and Yu[10] for their numerical computations in the laminar regime with uniform heating or cooling at the wall. The fixed parameters are Re = 400, Pr = 0.70, and K_{a0} = 0.096, for which Nu_{ox} = 6.2994, Sc = 0.20, E/RT_0 = 17.815, and T_0 = 300 K. The independent variables τ and J, the parameter ξ, and the dependent variables, Nu_x, T_{mx}/T_0, and k_{emx}/k_0 are included in Table 3 for reference. The values of β in Table 3 do not vary greatly despite a wide range of conditions as represented by a 10-fold variation in ξ and the enhancement of Nu_x by a factor of >25 for one set of conditions (τ = 0.05 and J = −0.05) and a factor of >4 for the converse condition (τ = −0.05 and J = 0.05). In this respect, Eq. 15 compares favorably with the analogies of Prandtl and Reichardt. However, δ^+ in the analogy of Prandtl is a function only of Re, and γ in the improved analogy of Reichardt is a function only of Re and the thermal boundary condition, whereas β is apparently a function of K_{x0}, τ, and J, and possibly of Re, Pr, K_{a0}, Sc, E/RT_0, and T_0 as well.

The dependency of β on K_{x0} is examined in Tables 4 and 5. Values of Nu_{xo}, corresponding to convection without reaction, are included as a point of reference for the enhancement of Nu_x by the reaction. In Table 4, the combination of τ = −0.01 and

Table 4. Selected Characteristics for Uniform Heating at Wall in Fully Developed Laminar Flow at Re = 400, Pr = 0.7, Sc = 0.2, K_{0a} = 0.096, τ = −0.01, J = 0.05, and ξ = −1.344

K_{0x}	Z_{mx}	Nu_x	T_{mx}/T_0	k_{mx}/k_0	$-Q_x$	β	β_{23}	Nu_{x23}
0.01	0.009853	24.844	0.99998	0.9995	1.330	0.0820	0.0453	23.55
0.02	0.019588	20.212	0.99995	0.9992	1.317	0.1013	0.0789	19.55
0.05	0.048104	15.487	0.99989	0.9981	1.290	0.1309	0.1238	15.33
0.10	0.09347	12.685	0.99981	0.9966	1.214	0.1569	0.1569	12.68
0.20	0.17713	10.360	0.99971	0.9948	1.100	0.1860	0.1905	10.42
0.50	0.38281	7.8202	0.99988	0.9981	0.828	0.2349	0.2349	7.820
1.00	0.61921	6.2691	1.00121	1.0225	0.523	0.2937	0.2685	6.173
2.00	0.86258	5.1198	1.00618	1.1171	0.206	0.4096	0.3021	4.998

Table 5. Selected Characteristics for Uniform Heating at the Wall in Fully Developed Laminar Flow at Re = 400, Pr = 0.7, $K_{a0} = 0.50$, $\tau = 0.05$, $J = -0.05$, and $\xi = -6.72$

K_{x0}	Z_{mx}	Nu_x	T_{mx}/T_0	k_{lmxe}/k_0	$-Q_x$	β	β_{24}	Nu_{x24}
0.01	0.009858	46.444	1.000421	1.00752	6.703	0.07809	0.07809	38.74
0.02	0.01965	48.585	1.000834	1.01495	6.686	0.09562	0.08808	42.62
0.03	0.02940	53.533	1.001247	1.02243	6.669	0.10712	0.10219	48.01
0.04	0.03910	59.590	1.001657	1.02991	6.650	0.11533	0.11220	54.70
0.05	0.04875	67.709	1.002066	1.03741	6.631	0.12209	0.11997	63.05
0.06	0.05836	78.089	1.002472	1.04491	6.612	0.12773	0.12631	73.64
0.07	0.06793	91.593	1.002876	1.05241	6.592	0.13259	0.13168	87.40
0.08	0.07745	109.70	1.003278	1.05993	6.571	0.13687	0.13632	105.9
0.09	0.08694	135.07	1.003677	1.06745	6.550	0.14066	0.14042	132.4
0.10	0.09635	172.83	1.004073	1.07495	6.528	0.14409	0.14409	172.9
0.20	0.18821	169.16	1.007922	1.15031	6.275	0.15160	0.16821	148.3
0.30	0.27508	92.184	1.011522	1.22498	5.967	0.15434	0.18233	82.85
0.40	0.35635	94.650	1.014841	1.29762	5.613	0.16554	0.19234	84.20
0.50	0.43155	161.35	1.017857	1.36690	5.222	0.18402	0.20010	140.2
0.60	0.50041	770.59	1.020556	1.43165	4.806	0.20645	0.20645	759.2
0.70	0.56283	90.259	1.022933	1.49093	4.380	0.21372	0.21182	79.85
0.80	0.61893	44.612	1.024994	1.54405	3.954	0.22125	0.21646	38.75
0.90	0.66893	28.826	1.027750	1.61772	3.599	0.22549	0.22056	26.35
1.00	0.71317	21.095	1.028218	1.63053	3.143	0.23814	0.22423	17.97
2.00	0.93597	6.6234	1.031918	1.73503	0.747	0.39134	0.24835	5.755

$J = 0.05$ is seen to result in a nearly invariant mixed-mean temperature until the conversion approaches unity and thereafter a linear increase. Apparently as a consequence of this near-isothermality, β increases monotonically with K_{x0} and produces a modest enhancement of Nu for all values of K_{x0}.

A plot by Yu and Churchill[10] of the numerically computed values of β vs. $\ln\{K_{x0}\}$ for all eight of the test conditions suggested the following empirical correlating equation:

$$\beta = A + B \ln\{K_{x0}\} \tag{22}$$

Evaluating the coefficients A and B for $\tau = -0.01$ and $J = 0.05$ at $K_{x0} = 0.1$ and 0.6 results in

$$\beta = 0.2585 + 0.04846 \ln\{K_{x0}\} \tag{23}$$

The representation of β by Eq. 23 is seen in Table 4 to be somewhat crude, but, as a fortuitous consequence of insensitivity, the resulting predictions of Nu_x are of sufficient accuracy for all practical purposes. The choice of other values of K_{x0} for the evaluation of the constants in Eq. 23 would result in different values of A and B but would not significantly change the overall accuracy of the predictions of β and Nu_x.

As illustrated in Table 5, the combination of $\tau = 0.05$ and $J = -0.05$ results in a monotonic increase in both T_{mx}/T_0 and β, but an extreme and irregular enhancement of Nu_x with increasing values of K_{x0}. The evaluation of the coefficients of Eq. 22 at the two peak values in Nu_x, that is, at $K_{x0} = 0.10$ and 0.60, results in

$$\beta = 0.2242 + 0.03480 \ln\{K_{x0}\} \tag{24}$$

The predictions of β by Eq. 24 are again somewhat crude and the corresponding predictions of Nu_x represent the chaotic behavior only semiquantitatively, but even that is quite an achievement for such a simple expression and is a strong endorsement of the validity of the structure of the analogy. On the other hand, the numerical difference in the coefficients of Eqs. 23 and 24 certifies the need for a correlative expression for β that incorporates the values of τ and J, even for fixed values of Re, Pr, K_{0a}, Sc, E/RT_0, and T_0, if the analogy is to be predictive in a numerical sense.

Turbulent flow with uniform heating and cooling

Table 6 illustrates the variance of β at $K_{x0} = 0.5$ for turbulent flow at Re = 37,640, but otherwise the same eight conditions as for Table 3; however, the results differ dramatically. Not only is the numerical variance of β much greater, but the sign is negative for four of the conditions. In the quest for less invariance and an explanation for the differences relative to Table 3, finite-difference computations were carried out by

Table 6. Variance of Coefficient β at $K_{x0} = 0.50$ with Thermicity and Heat Flux Density Turbulent Flow at Re = 37,640 and Pr = 0.7, for Which $\mathrm{Nu}_{ox} = 107.69$, Sc = 0.2, $E/RT_0 = 17.815$, and $T_0 = 300$ K

τ	J	$-\xi$	Z_{mx}	Nu_x	T_{mx}/T_0	k_{emx}/k_0	β
0.01	−0.05	126.47	0.40280	190.069	1.00399	1.07334	0.005346
−0.01	0.05	126.47	0.38008	251.529	0.99624	0.93495	0.007801
0.01	−0.10	63.235	0.40264	478.960	1.00395	1.07256	0.01913
−0.01	0.10	63.235	0.38023	386.759	0.99628	0.93559	0.01968
0.05	−0.05	632.35	0.46001	11.8638	1.02296	1.49033	−0.01587
−0.05	0.05	632.35	0.34199	22.3052	0.98294	0.73404	−0.01253
0.05	−0.10	316.18	0.45981	27.0058	1.02291	1.49037	−0.01173
−0.05	0.10	316.18	0.34211	55.3732	0.98274	0.73449	−0.006185

Table 7. Selected Characteristics for Uniform Heating at the Wall in Fully Developed Turbulent Flow at Re = 37,640, Pr = 0.7, Sc = 0.2, $K_{a0} = 0.096$, $\tau = -0.01$, $J = 0.05$, and $\xi = -126.47$

K_{x0}	Z_{mx}	Nu_{xo}	Nu_x	T_{mx}/T_0	k_{emx}/k_0	$-Q_x$	β	β_{26}	Nu_{x26}
0.010	0.009932	250.95	2032.96	0.99990	0.99824	124.99	0.007012	0.007012	2033
0.020	0.019743	204.35	3486.72	0.99900	0.99652	123.54	0.007620	0.007688	4070
0.030	0.029435	182.70	1079.43	0.99971	0.99481	122.11	0.006803	0.007474	2092
0.040	0.039011	169.56	684.72	0.99961	0.99311	120.68	0.006234	0.007098	1183
0.050	0.048473	160.53	522.50	0.99952	0.99147	119.31	0.005806	0.006705	802.7
0.060	0.057823	153.86	434.07	0.99942	0.98983	117.95	0.005473	0.006336	608.9
0.070	0.067062	148.67	378.49	0.99934	0.98821	116.60	0.005208	0.006001	495.1
0.080	0.076193	144.49	340.41	0.99924	0.98662	115.27	0.004993	0.005704	421.9
0.090	0.085218	141.03	312.79	0.99922	0.98617	114.09	0.004813	0.005442	372.0
0.10	0.094111	138.11	291.98	0.99907	0.98350	112.68	0.004677	0.005216	335.0
0.20	0.17785	122.26	215.78	0.99824	0.96903	100.76	0.004301	0.004301	215.8
0.30	0.25268	115.12	207.80	0.99750	0.95628	90.38	0.004935	0.004876	218.6
0.40	0.31977	110.75	221.38	0.99683	0.94499	81.30	0.006147	0.006262	226.6
0.50	0.38009	107.69	251.53	0.99624	0.93495	73.30	0.007801	0.008164	262.4
0.60	0.43447	105.39	302.73	0.99570	0.92600	66.23	0.009842	0.010428	340.7
0.70	0.48358	103.57	389.83	0.99522	0.91799	59.96	0.012248	0.012959	464.2
0.80	0.52804	102.07	555.27	0.99478	0.91080	54.37	0.015013	0.015698	596.4
0.90	0.56834	100.82	966.35	0.99439	0.90434	49.37	0.018142	0.018604	1237
1.00	0.60492	99.75	3539.98	0.99410	0.89853	44.90	0.021646	0.021646	3537
2.00	0.83281	93.87	180.61	0.99183	0.86451	19.26	0.024937	0.056405	94.0
5.00	0.98596	89.49	93.59	0.99054	0.84348	1.497	0.029258	0.176905	121.7

Yu and Churchill[10] for 16 additional conditions, primarily involving greater absolute values of the dimensionless heat flux density J, although herein attention is confined to the conditions of Table 6. As can be deduced from Eq. 7, the negative values of β arise from the attenuation of Nu_x relative to Nu_{ox}. The difference in the values of β in Tables 3 and 6 indicates that the dependency on Re is not wholly characterized by its presence in ξ, at least insofar as one condition is in the laminar regime and the other is in the turbulent regime. This discrepancy might have been anticipated because the turbulent transport of energy and species is accounted for in Eq. 8 only by virtue of the presence of $(k_{emx}/k_0)(1 - Z_{mx})$.

Tables 7 and 8, which illustrate the dependency of Nu_x, β, and other dependent variables on K_{x0} and which include Nu_{ox} as a reference, constitute a counterpart to Tables 4 and 5. In the turbulent regime, Nu_{ox} depends separately on Re, Pr, and a/x rather than on $\mathrm{Gz} = \pi\mathrm{RePr}a/x$ only. Thus these values of Nu_{ox} are specific to the indicated conditions. All eight pairs of values of τ and J resulted in one or two peaks in Nu_x and a nonmonotonic dependency of β on K_{x0}.

The behavior for $\tau = -0.01$ and $J = 0.05$ is summarized in Table 7. Because β goes through a minimum as K_{x0} increases, Eq. 22 is obviously inadequate, and the following expression is proposed as an alternative:

$$\beta = A + B\left(\ln\{K_{x0}\} - \frac{K_{x0}}{K_{x0c}}\right) + C\left(\ln\left\{\frac{K_{x0}}{K_{x0c}}\right\}\right)^2 \qquad (25)$$

Equation 25 was formulated to result in $d\beta/dK_{x0} = 0$ at $K_{x0} = K_{x0c}$, which is at the minimum in β, and presumably in Nu_x as well, and, by virtue of the squared term, to accommodate some deviation from the semilogarithmic dependency. The values of A, B, and C were evaluated from the calculated values of β for $K_{x0} = 0.01$, 0.2, and 1.0, and K_{x0c} was taken to be 0.2, resulting in

$$\beta = -0.01971 - 0.009201\left(\ln\{K_{x0}\} - \frac{K_{x0}}{0.20}\right) - 0.001795\left(\ln\left\{\frac{K_{x0}}{0.20}\right\}\right)^2 \qquad (26)$$

The accuracy of the predictions of β by Eq. 26 is seen in Table 7 to be only fair, but the resulting predictions of Nu_x are

Table 8. Selected Characteristics for Uniform Cooling at the Wall in Fully Developed Turbulent Flow at Re = 37,640, Pr = 0.7, Sc = 0.2, $K_{a0} = 0.096$, $\tau = 0.05$, $J = -0.05$, and $\xi = -632.3$

K_{x0}	Z_{mx}	Nu_{xo}	Nu_x	T_m/T_0	k_{emx}/k_0	$-Q_x$	$-\beta$	$-\beta_{27}$	Nu_{x27}	$-\beta_{28}$	Nu_{x28}
0.01	0.009988	250.95	71.8160	1.000499	1.0089	631.62	0.003949	0.003949	71.82	0.4873	0.813
0.02	0.019962	204.35	45.0698	1.000997	1.0179	630.81	0.005602	0.005973	42.86	0.3153	1.022
0.05	0.049800	160.54	26.0508	1.002486	1.0452	628.00	0.008221	0.008648	24.96	0.1515	1.670
0.10	0.099135	138.12	18.2220	1.004948	1.0917	621.90	0.010580	0.010672	18.09	0.07353	2.955
0.20	0.19591	122.26	13.6241	1.009780	1.1883	604.22	0.013201	0.012695	14.10	0.03112	6.173
0.50	0.45001	107.69	11.8638	1.022961	1.4790	514.37	0.015703	0.015371	12.09	0.01598	11.68
0.60	0.53593	105.39	12.5120	1.026749	1.5906	466.77	0.015903	0.015903	12.51	0.01590	12.51
0.70	0.60467	103.57	13.6226	1.030178	1.6852	421.27	0.015673	0.016353	13.13	0.01584	13.50
0.80	0.66598	102.07	15.2455	1.033236	1.7737	374.63	0.015202	0.016742	14.04	0.01550	14.99
0.90	0.71989	100.82	17.4871	1.035923	1.8490	328.54	0.014505	0.017087	15.24	0.01476	17.23
1.00	0.76667	99.75	20.5211	1.038254	1.9278	284.44	0.013573	0.017394	16.77	0.01357	20.52
2.00	0.96989	93.87	930.543	1.048336	2.2737	43.291	−0.02077	0.019418	51.00	−0.02077	931.42
5.00	0.99996	89.49	89.6433	1.049603	2.3208	0.059	−0.02883	0.022093	89.38	−0.07470	88.18

Table 9. Variance of β at $K_{x0} = 0.50$ with τ and T_w/T_0 Laminar Flow at Re = 400 with Pr = 0.7, for Which $Nu_{ox} = 5.0383$, Sc = 0.2, $E/RT_0 = 17.815$, and $T_0 = 300$ K

τ	T_w/T_0	Z_{mx}	Nu_x	T_{mx}/T_0	k_{emx}/k_0	J_x	$-\xi_x$	β
0.01	1.00	0.38492	13.289	1.00268	1.04871	−0.01779	3.7774	0.25481
0.05	1.00	0.41901	12.903	1.01476	1.29568	−0.09519	3.5298	0.22938
−0.01	1.00	0.37040	13.467	0.99744	0.99511	0.26820	3.8808	0.26820
−0.05	1.00	0.34521	13.799	0.98819	0.80821	0.08149	4.1231	0.29096
0.01	0.90	0.27955	5.1173	0.97842	0.67506	−0.20065	0.3349	0.09483
0.05	0.90	0.30392	5.4038	0.98852	0.81312	−0.23918	1.4048	0.08509
−0.01	1.10	0.51921	5.5473	1.02089	1.43981	0.21942	0.3062	0.43285
−0.05	1.10	0.48885	7.2756	1.01203	1.19713	0.32666	1.0286	0.48857

perhaps, in consideration of the erratic behavior, of acceptable accuracy.

For $\tau = 0.05$ and $J = -0.05$, as shown in Table 8, β is negative for $K_{x0} \leq 1.0$ by virtue of $Nu_x \leq Nu_{x0}$, and goes through a maximum in absolute value at $K_{x0} = 0.60$. On the other hand, Nu_x goes through a maximum at $K_{x0} = 2.0$. The behavior of β for $0.01 \leq K_{x0} \leq 0.60$ may be represented reasonably well by the following interpolative expression:

$$-\beta = 0.01739 + 0.02919 \ln\{K_{x0}\} \tag{27}$$

The corresponding values of Nu_x in that range of K_{0x} are seen to be of acceptable accuracy. The values of β for $0.6 \leq K_{0x} \leq 1.0$, on the other hand, are well represented by the following expression based on the values of K_{0x} at 0.60, 1.0, and 2.0, and the location of the minimum at 0.60:

$$-\beta = 0.1519 + 0.09\left(\ln\{K_{x0}\} - \frac{K_{x0}}{0.60}\right) + 0.04482\left(\ln\left\{\frac{K_{x0}}{0.60}\right\}\right)^2 \tag{28}$$

The predictions of Nu_x by Eq. 28, including the peak value, are seen to be in almost exact agreement with the values computed by finite differences. A correlating equation for all values of K_{x0} could readily be constructed either by a combination of Eqs. 27 and 28 or by an alternative more complex expression. However, such a construction has very limited utility because it merely reproduces the computed values of β and Nu_x for a particular set of conditions and has no generality.

Uniform wall temperature

The values of β for uniform wall temperatures were calculated from Eq. 20 using the values of Nu_x, Z_{mx}, and T_{mx}/T_0 computed by Yu and Churchill.[11] Values for $K_{x0} = 0.50$ are listed in Table 9 for a laminar flow and in Table 10 for a turbulent flow. The values of β are relatively invariant with respect to τ in each regime of flow, but vary strongly with the chosen values of T_w/T_0. In laminar flow, the Nusselt number is attenuated slightly for $T_w/T_0 = 1.0$ and strongly for both higher and lower ratios. In turbulent flow, the Nusselt number is appreciably enhanced for $T_w/T_0 = 1.0$ and slightly for other ratios. Anomalous behavior, including peak values in Nu_x, did not occur for any of the chosen conditions. Values of β computed from Eq. 20 vary monotonically with K_{x0} and the behavior in each case could be represented by Eq. 22, although this was not done because a supplementary correlation for T_{mx}/T_0 would be required to predict Nu_x.

Interpretation

The objective of the work reported here was to devise an analogy between chemical reaction and convective heat transfer. That objective has been accomplished but the results appear to open as many doors as they close. This section is focused on these unresolved issues in two categories. First, the proposed analogy is compared with classical analogies for momentum and heat transfer. Second, the utility of the new analogy is examined vis-à-vis the finite-difference solution of the PDEs of conservation.

Comparison of the new analogy for reaction and convection with the classical analogies for momentum and heat transfer

Derivations of the classical analogies for momentum and heat transfer have been described above and need not be repeated here. These analogies have played a significant role in practice in that they have provided models for both correlation and prediction. The analogy of Colburn[3] is still widely used despite its numerical and functional inaccuracy. The derivation of the analogy of Reichardt[4] provides great functional insight, and its recent reformulation by Churchill and Zajic[6] is so nearly exact numerically and functionally that it may remain competitive with numerical simulations as they become standard practice.

Table 10. Variance of β at $K_{x0} = 0.50$ with τ and T_w/T_0 Turbulent Flow at Re = 37,640 with Pr = 0.7, for Which $Nu_{ox} = 103.51$, Sc = 0.2, $E/RT_0 = 17.815$, and $T_0 = 300$ K

τ	T_w/T_0	Z_{mx}	Nu_x	T_{mx}/T_0	k_{emx}/k_0	J_x	$-\xi_x$	β
0.01	1.00	0.40237	157.529	1.00385	1.07076	−0.30344	20.840	0.02571
−0.01	1.00	0.38047	158.829	0.99636	0.93700	0.28902	21.879	0.02742
0.05	1.00	0.45636	154.501	1.02189	1.46470	−1.69117	18.696	0.02217
−0.05	1.00	0.34399	161.156	0.98358	0.74267	1.32347	23.890	0.03073
0.01	0.90	0.38500	104.261	0.99902	0.99275	−1.22497	5.1622	0.00971
0.05	0.90	0.43632	106.955	1.01647	1.33457	−6.22855	5.0762	0.00843
−0.01	1.10	0.40254	107.622	1.00095	1.01708	5.32988	1.1864	0.05297
−0.05	1.10	0.36437	121.204	0.98776	0.80197	6.80176	4.6484	0.06160

The new analogy superficially resembles classical analogies in that the Nusselt number is predicted on the basis of the behavior of another quantity—the mixed-mean conversion in the case of chemical reaction and the friction factor in the case of momentum transfer. The similarity largely ends there. To begin with, classical analogies relate the transport of two different quantities, momentum and energy, whereas the new analogy relates a generative process to one of transport. Mathematically, two vectorial quantities are related in the classical analogies but a vectorial quantity and a scalar quantity are related in the new analogy. Moreover, classical analogies relate two fully developed processes, whereas the new analogy relates two developing processes. Classical analogies apply only for turbulent flow, whereas the new analogy is applicable for both laminar and turbulent flows. The function γ in the modified Reichardt analogy represents a well-defined integral but the coefficient β in the new analogy is an unknown function of several variables. Some insight is gained by examining the sources of these differences.

Because of the fundamental differences mentioned in the preceding paragraph, the derivation of the new analogy followed a completely different procedure than that used for any of the classical analogies. First, an exact solution for heat transfer was derived for a notably idealized case of fully developed convection and reaction. That solution was then adapted for devolving reaction and developing convection by replacing the theoretical coefficient of linking with an arbitrary one, and introducing an arbitrary expression for the effective mean value of the reaction-rate constant with respect to both radius and axial distance at each value of K_{ox}.

The analogy for uniform heating was adapted speculatively for a uniform wall temperature simply by replacing the specified heat flux density by the (unknown) local value and then, by virtue of the definition of the local Nusselt number, replacing that unknown quantity by another unknown quantity, that is, the mixed-mean temperature ratio T_{mx}/T_0. The result is inferior to that for a uniform heat flux in the sense of numerical predictions because it includes this ratio as well as the mixed-mean conversion and the arbitrary coefficient β. However, it appears to have similar merit in a structural sense.

Chemical reaction and convection in tubular flow are ordinarily developing processes, whereas convection in the absence of chemical reaction and in a long tube with either a uniform heat flux density or a uniform wall temperature approaches a fully developed dimensionless state and may be considered to be fully developed throughout to a good degree of approximation. Thus, that difference in the new and classical analogies in that respect simply conforms to practice. The coefficient β in the new analogy is a function of the dimensionless distance from the entrance because the reaction and convection are progressing, whereas the friction factor f in the classical analogies is not, given that the flow and the convection are presumed to be fully developed. The coefficient β is also a function of the thermicity and the heat flux density because the temperature and the rate of reaction are varying with distance from the entrance.

An analogy has apparently not been formulated between momentum and convective heat transfer in developing convection in fully developed laminar flow because the classical solutions of Graetz[12] in series form are a function only of $wc/\lambda x = (\pi a/2x)\mathrm{RePr}$ and the thermal boundary condition, and are independent of the friction factor as a separate variable. Of course, $16/f$ could be substituted for Re to give the appearance of an analogy. For fully developed convection, these solutions of Graetz reduce to a fixed value for Nu (in the case of a uniform heat flux density to the value of 48/11 of Eq. 5) and remain independent of the friction factor.

The derivation of the analogy and the test computations are for a first-order equimolar irreversible reaction. These are unnecessarily severe restrictions in that a pseudo first-order rate mechanism, together with an effective frequency factor, energy of activation, heat of reaction, and molecular weight, could be used to approximate the net effect of multiple reactions on the Nusselt number.

In summary, the new analogy differs fundamentally from classical analogies in that it links two dissimilar processes and has a much broader scope, encompassing both developing and fully developed convection and reaction in both laminar and turbulent flows. The price of that difference and of the broader scope is a dependency of the coefficient β on many variables as compared to the dependency of δ^+ in the analogy of Prandtl on the Reynolds number alone, and the dependency of γ in the modified analogy of Reichardt on the Reynolds number and mode of heating alone. Whereas the latter modified analogy of Reichardt, together with numerically computed values of γ, provides almost exact numerical predictions of the Nusselt number for fully developed convection in fully developed turbulent flow for all Re and Pr and both modes of heat transfer, the predictive power of the new analogy is, as illustrated in Tables 4, 5, 7, and 8, limited to one case at a time.

An Explanation for the Enhancement and Attenuation

The analogy, in the generic form of Eq. 7, as well as in the detailed form of Eqs. 15 and 21, provides a representation for the enhancement and the attenuation of the Nusselt number, including the extreme and chaotic values. For example, the extreme enhancement is a result of $Q_x\beta \rightarrow 0$, and the chaotic behavior is a serendipitous result of the independent variations of Q_x and β, although this does not constitute a physical explanation. Although Eq. 8 provides essentially exact values of Q_x in terms of the specified variables, the dependency of β on these same quantities has yet to be formulated either analytically or computationally.

A physical explanation was conjectured on the basis of the modification of the radial temperature distribution by the heat of reaction, whose generation depends on the local temperature and composition, which in turn depend critically not only on the velocity distribution, but also on the Prandtl and Schmidt numbers. The preferential generation of the heat of reaction near the wall shifts the mixed-mean temperature toward the wall, reducing the mean distance for the transfer of this energy to the wall as compared to the mean distance in the case of pure convection and thereby enhancing Nu_x. Attenuation is conversely a result of preferential generation of the heat of reaction near the centerline. The temperature distributions computed by Yu and Churchill[10] for uniform heating with and without reaction confirm this conjecture for both laminar and turbulent flows.

The Role of Simulation

One alternative to the use of a correlating equation—irrespective of whether it is in the form of an analogy—for the prediction of flow, heat transfer, mass transfer, and/or a chemical conversion is the numerical solution by finite-difference methods of a mathematical model in the form of the PDEs of conservation for momentum, energy, and chemical species. The continual development of improved computer hardware and software expands the range of behavior that is within the reach of undergraduate students and practicing engineers by such methodologies. A brief review of the state of the art of such computations would appear to be an essential point of reference for the evaluation of the present and future role, if any, of analogies.

Numerical solutions for fully developed flow, either laminar or turbulent, in a round tube, a parallel-plate channel, or a concentric circular channel, are within the grasp of undergraduate students and practitioners in chemical, mechanical, and aerospace engineering, although supplementary tutoring may be required with respect to transport by the turbulent fluctuations. Exact algebraic solutions in closed form exist for the friction factor in laminar flow and accurate algebraic correlating equations for turbulent flow, but a finite-difference computation may be more convenient if a solution for forced convection, with or without chemical reaction, is to be carried out simultaneously. Computer packages provide a third alternative.

Numerical solutions by finite-difference methods for pure, developing, forced convection in fully developed flow are also within the reach of undergraduate students and practitioners in chemical, mechanical, and aerospace engineering. For the laminar regime, the execution of such solutions requires less programming and less computation for a given degree of accuracy than the classical solutions of Graetz in the form of infinite series. For the turbulent regime, the analogy of Reichardt as modified by Churchill and Zajic may be of sufficient accuracy, although the finite-difference formulation proved to require less computation and to be more accurate for determination of the values of Nu_{ox} and Nu_{oxT} used herein. Computer packages may again provide a third alternative.

When chemical reactions are carried out in fully developed tubular flow, momentum transfer generates a velocity distribution and thereby, for all but a zero-order reaction, a radial distribution in composition. The resulting concentration gradients generate mass transfer. The velocity distribution also generates a radial temperature gradient for all energetic reactions and thereby radial heat transfer. The analytical solution could be used for the velocity distribution in fully developed laminar flow and a correlating equation for fully developed turbulent flow, but the simultaneous solution of the PDE for the conservation of momentum with PDEs for the conservation of energy and species is again more efficient computationally. These solutions are within the reach of undergraduates and most practitioners in chemical engineering. This is not an idle assertion; such modeling and computations are illustrated by Churchill and Yu.[9] However, computer packages for reacting flow for even the simplest of conditions are yet in a state of development.

The postulate of fully developed flow implies that entrance effects are negligible and, in the case of heat transfer, that changes in the density, viscosity, thermal conductivity, and heat capacity are negligible as well. In the case of chemical reaction, changes in these several properties with composition, and of the heat of reaction with temperature must also be considered negligible to support the postulate of fully developed flow. Molecular and eddy diffusion of energy and species in the direction of flow are commonly postulated to be negligible. Accounting for these effects significantly complicates the modeling and perhaps beyond the reach of both undergraduates and practitioners.

In the interests of simplicity, all of the derivations herein have been confined to a single first-order or zero-order, irreversible, equimolar reaction. Even for this simple case, accounting for the dependency of the reaction rate on temperature is essential; this was done rigorously in the supporting computations of Yu and Churchill[10,11] and approximately by means of Eq. 12 in the analogy. Multiple reactions complicate but do not change the character of the modeling by adding additional equations for the conservation of species and terms for the conservation of energy, whereas nonequimolar reactions change the density and thereby the velocity field both radially and longitudinally. Both the modeling and the numerical computations for such complex schemes of reaction may stretch the capabilities of both undergraduates and practicing engineers. However, help in the form of computer packages should soon be at hand.

On the basis of the above analysis, numerical simulation would appear to have an essential role in education and practice in fluid mechanics, heat transfer, mass transfer, and reaction engineering. It actually has a pervasive and growing role in all but reactor engineering, where education and practice in this respect appear to be frozen in the past. Despite the existing skill of the students, methodologies and solutions that take into account simultaneous momentum, energy, and mass transfer for chemical conversions in tubular flow are not to be found in the textbooks on reaction engineering or in the packages for computer-aided design. Instead, the solutions and methodologies are based on the concept of "plug flow," which obviates the consideration of momentum, mass, and energy transfer at the price of an error of unknown magnitude.

The Role of Experimentation

Experimentation is the ultimate standard for the evaluation of the accuracy of both simulations and theoretical expressions such as analogies. However, heat transfer and reaction engineering are currently out of favor as subjects of research in the laboratory. The only direct measurements of enhancement arising from a reaction that were identified are those Edwards and Ferguson[13] for the gas-phase decomposition of oxone in turbulent flow through a uniformly heated glass tube. Their observations of enhancements of up to 27% are consistent with the predictions of Eq. 15, but insufficient information is given to make quantitative comparisons.

The Role of the Proposed Analogy between Chemical Reaction and Convection

In consideration of its limitations with respect to numerical predictions and the potential of finite-difference solutions, what role, if any, does the analogy derived herein serve?

This analogy has already made a unique and invaluable

contribution by providing the first quantitative explanation for the chaotic and extreme enhancement and attenuation of convection by an energetic reaction. An explanation of this anomalous behavior would not be easy to discern from the numerical results of simulation and/or experimentation, however extensive.

A further unique contribution of the new analogy has been to identify the variables and parameters that influence the combined process of reaction and convection, such as those that make up Eqs. 15 and 20. Although the indicated functional dependency of Nu_x on these several dimensionless groupings may not be exact because of the speculations and approximations used in the derivations, even first-order prediction of their effects is invaluable and provides a guide to simulation and experimentation.

Another important but fuzzy contribution is the numerical prediction of Nu_x as a function of Z_{mx}. The explicit empiricism within Eqs. 15 and 20 is limited to the coefficient β, but, as contrasted to the arbitrary functions such as δ^+ and γ in the analogies for momentum and heat transfer, a generalized and comprehensive predictive expression or correlating equation for that coefficient has not as yet been developed. The variation of β with the dimensionless distance through the reactor, K_{x0}, was found to be regular and moderate and to be represented successfully by a linear and/or a quadratic expression in $\ln\{K_{x0}\}$ even for conditions for which Nu_x varies chaotically and grossly. That is a significant, if incomplete, achievement in that the empirical coefficients in these correlating equations are unknown functions of the thermicity ($\tau = q_M/c_M T_0$), the dimensionless heat flux density ($J = j_w a/\lambda T_0$), or the wall-temperature ratio (T_w/T_0), the regime of flow (laminar or turbulent), and possibly some of the factors that make up ξ, ξ_x, and ζ. This uncertainty is a consequence of the speculative derivation of the new analogy and is a direct counterpart of the uncertainty with respect to the dependency on Pr in the classical analogies.

Summary and Conclusions

A relationship between the mixed-mean conversion and the Nusselt number has been derived for a homogeneous energetic chemical reaction in tubular flow with compensatory heat exchange.

This relationship can be interpreted as an analogy in the sense of the well-known interrelation between momentum and heat transfer.

Counterparts of the classical analogies and the new analogy are, respectively:

Dependent Variable

- Nusselt number for fully developed turbulent convection
- Local Nusselt number for developing laminar or turbulent convection

Independent Variable

- Fanning friction factor for fully developed turbulent flow
- Local mixed-mean conversion for a devolving reaction in fully developed laminar or turbulent flow

Parameters

- Nominal coefficient of unity in the Reynolds and Colburn analogies, δ^+ in the Prandtl analogy, and γ in the modified Reichardt analogy
- The coefficient β

The new analogy thus has a broader scope than that of the classical analogies in that it encompasses devolving reaction and developing convection and both laminar and turbulent flow, but it is inferior in terms of absolute predictions because, as a consequence of the many parameters associated with a chemical conversion and heat exchange, a generalized expression has yet to be developed for the empirical coefficient β.

Although the derivation herein is based on a single, irreversible, equimolar reaction it is applicable as an approximation for any reactive process in terms of an effective rate constant, heat of reaction, and mean density.

The principal merits of the new analogy are the explanation of the chaotic and gross variation of the Nusselt number and the quantitative prediction of that behavior for any single condition.

The main shortcoming of the analogy is the absence of a generalized predictive or correlative expression for the coefficient β. Progress in this respect is currently limited to the observation of a limited variance for different thermal conditions and a nearly semilogarithmic dependency on distance through the reactor/exchanger.

Notation

a = radius of tube, m
A = an arbitrary constant
B = an arbitrary constant
c = specific heat capacity, J kg^{-1} K^{-1}
C_M = molar heat capacity, J kg^{-1} mol^{-1} K^{-1}
C_{A0} = initial molar concentration of reactant A
D_f = diffusivity of species A, m^2/s
E = energy of activation, J kg-mol^{-1}
f = Fanning friction factor; $2\tau_w/\rho u_m^2$
Gz = Graetz number; $wc/x\lambda = (\pi a/2x)$RePr
j_w = heat flux density in the y-direction, W/m^2
J_x = dimensionless local heat flux density from wall; $aj_w/\lambda T_0$
J = dimensionless uniform heat flux density from wall; $aj_w/\lambda T_0$
k = reaction rate constant, s
K_{a0} = dimensionless rate of reaction; ak_0/u_m
K_{x0} = dimensionless distance from entrance; xk_0/u_m
Nu = Nusselt number; $2aj_w/\lambda(T_w - T_m)$
Pr = Prandtl number; $c\mu/\lambda$
Pr$_t$ = turbulent Prandtl number
q_M = molar heat of reaction, J kg-mol^{-1}
Q = ratio of heat of reaction to heat flux from wall; $ak_0C_{A0}(1 - Z_m)q_M/2j_w$
R = Rydberg constant, J kg-mol^{-1} K^{-1}
Re = Reynolds number; $2au_m\rho/\mu$
Sc = Schmidt number; $\mu/\rho D_f$
T = absolute temperature, K
u_m = mixed-mean velocity, m/s
w = mass rate of flow, kg/s
Z = fractional conversion of reactant A

Greek letters

β = arbitrary coefficient in analogy for reaction and heat transfer
γ = integral function of velocity and temperature distributions (see Churchill and Zajic[7])
δ = boundary layer thickness, m
$\delta^+ = \delta(\tau_w\rho)^{1/2}/\mu$
$\zeta = \tau$RePr$K_{a0}/2$
η = arbitrary exponent
λ = thermal conductivity, W/mK
μ = dynamic viscosity, kg m^{-1} s^{-1}
$\xi = \tau$RePr$K_{a0}/4J$
ρ = specific density, kg/m^3
τ = thermicity; $q_M/c_M T_0$

Subscripts

c = at minimum or maximum in β
e = effective mean
m = mixed mean
o = for no reaction
T = for uniform wall temperature
w = at wall
x = local value at distance x from inlet
0 = at entrance

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