AN ANALOGY BETWEEN REACTION AND HEAT TRANSFER

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Abstract

The most accurate predictions of forced convection in fully developed turbulent flow are produced by modifications and generalizations of the Reichardt analogy between momentum and energy transfer. That analogy was originally derived by combining the differential energy and momentum balances, making several ingenious mathematically based approximations, introducing an algebraic model for turbulent transport, and finally integrating over the radius in closed form. Subsequent improvements have resulted from the introduction of a better model for transport by the turbulent fluctuations.

A comparable analogy between convective heat transfer and an energetic chemical conversion has been devised by a completely different process of modeling. First, an exact algebraic solution was derived for convection in fully developed laminar flow with a volumetrically uniform rate of reaction and no radial diffusion of species. That solution, which relates the Nusselt number to the ratio of the heat flux at the wall to the heat of reaction, was then generalized for developing reaction and convection, including diffusion, at the expense of the introduction of one functional idealization and one arbitrary coefficient. The error due to the functional idealization, which consists of expressing the rate of reaction in terms of the mixed-mean temperature, appears to be completely negligible. The arbitrary coefficient, which was evaluated by means of essentially exact numerical computations, proved to vary regularly and moderately from condition to condition and thereby to be susceptible to correlation and generalization.

The new analogy incorporates an explicit dependence on *Re*, *Pr*, *Sc*, as well as on a number of other dimensionless parameters involving the frequency factor, the energy of activation, and the thermicity of the reaction, the heat flux density or the temperatre at the wall. It is applicable for both laminar and fully turbulent flow. In combination with a complementary expression for the chemical conversion, the analogy becomes predictive in a numerical sense. The resulting predictions have been tested by comparison with essentially exact numerical solutions, and have proven satisfactory even for conditions that produce gross and seemingly chaotic enhancement or attenuation of the Nusselt number.

The success of this analogy as well as the improved one of Reichardt suggests that similar theoretically structured expressions may be possible for other processes involving transport and/or reaction.

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 run-away.

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 due to 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.

Two thermal boundary conditions are considered, first a uniform heat flux density through the wall of the tube, and second 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 with out 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 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 most chemical processes involve multiple reaction mechanisms, each of which depends exponentially and differently on temperature, and many of which are non-equimolar. The general model for combined reaction and heat transfer consists of a set of partial differential equations for the conservation of species that are nonlinear in temperature, generally nonlinear in concentration, and strongly coupled with the partial differential equation 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 are neglected, may be modeled by a single linear partial differential equation, 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. On the other hand the radial transport of momentum, energy, and species are taken into account.

To meet the limitations of this format on length a listing of the nomenclature and some of the tabulations of the computed values have been omitted. They will be included in a subsequent publication in the *AIChE Journal*.

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, Prandtl, and Colburn. They are all three well-known and will not be described herein. Reichardt[1] in 1950 derived a greatly improved analogy that is less well known although it provides the structure for many correlating equations. 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, in order 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[2] for a discussion thereof). As an example of such modifications, Churchill and Zajic[3] not only improved upon 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:

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

Here, γ is a theoretically defined integral that depends mildly on *Re*, Pr_t/Pr, and the thermal boundary condition at the wall.

All of the afore-mentioned analogies, including Eq. (1), are limited in applicability to large and moderate values of *Pr*, but Churchill and Zajic also devised a an expression equivalent to Eq. (1) for $Pr \leq Pr_t \cong 0.86$, which need not be reproduced here.

The purpose of this digression is to serve as a guide and point of referral for the derivations that follow for the combination of an energetic chemical reaction and heat exchange. In order to avoid excessive expectations for an analogy between reaction and heat transfer, it should be noted that implementation of the Reichardt analogy, as well as those of Reynolds, Prandtl, and Colburn, 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, 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, as well as a theoretically based function, namely $\gamma\{Re,Pr$, 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[4] of an exact solution in closed form for a very idealized process of flow, reaction, and heat transfer, namely 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 the radial diffusion of species. A volumetrically uniform rate of reaction might be rationalized on the basis of asymptotically small perturbations in the composition due to the reaction and in the temperature due to the combination of the heat of reaction and the imposed heat flux. In any event, the solution can be expressed as

$$Nu = \frac{48/11}{1+3Q/11} \tag{2}$$

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 $Q \rightarrow 0$, $Nu \rightarrow 48/11$, 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. (2) to decrease slowly as Q increases. Eq. (2) 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. (2) for positive and negative values of Q are given credence by their qualitative congruence with prior theoretical and experimental predictions of enhancement and attenuation due to energetic reactions. Most important, Eq. (2) 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. (2) for laminar flow. However, it may be speculated that the form of Eq. (2) 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

$$Nu = \frac{Nu_o}{1+\beta Q} \tag{3}$$

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. (3), enhancement and attenuation of Nu are characterized by the product βQ.

Eq. (3) 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. (2) was derived. The corresponding values of β not only differ from the fixed value for laminar flow, but reveal a moderate dependence on Re and Pr. This dependence is disappointing, but that disappointment is assuaged by the complete

independence of β from the parameter Q. Since 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.

Adaptation of the Analogy for Developing Reaction and Convection

Eqs. (2) and (3) 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. (3) was rewritten as follows for the much more complex and realistic case of developing reaction and developing convection:

$$Nu_x = \frac{Nu_{ox}}{1+\beta Q_x} \tag{4}$$

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 convection is Nu_x/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 expressed as follows:

$$Q_x = \frac{\pi a^2 C_{A0}(1-Z_{mx})kq_M}{2\pi a j_w} = \frac{\tau \,\mathrm{Re}\,\mathrm{Pr}\, K_{a0}(1-Z_{mx})}{4J} = \xi(1-Z_{mx}) \tag{5}$$

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; $K_{a0} = k_0 a/u_m$ is the dimensionless rate of reaction; $\tau = q_M/c_M T_0$ is the *thermicity*, that is the increase in temperature due to an exothermic reaction ($q_M > 0$) or the decrease due an endothermic one ($q_M < 0$); 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 a dependent variable. The factor $\xi \equiv \tau RePrK_{a0}/4J$ is a combination of the specified variables in Eq. (5), namely 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. (5) 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. (5) is proposed. First, the dependence of the reaction–rate constant on temperature is postulated to be given by the Arrhenius equation, namely,

$$k = k_\infty e^{\frac{-E}{RT}} = k_0 e^{\frac{E}{RT_0}\left(1-\frac{T_0}{T}\right)} \tag{6}$$

The right–most form of Eq. (6), which was apparently first introduced by Churchill[8] is utilized 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. (6), 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, in order to take the variation of the reaction–rate constant according to Eq. (6) into account in the reactor, the right-most form of Eq. (5) is re-expressed as

$$Q_x = \left(\frac{k_{emx}}{k_0}\right)\xi\,(1-Z_{mx}) \tag{7}$$

Here k_{emx} is the effective–mean value of the rate constant over the cross-section at x. With these supplementations, Eq. (4) can be re-expressed as

$$Nu_x = \frac{Nu_{xo}}{1+\beta\left(k_{emx}/k_0\right)\xi\left(1-Z_{mx}\right)} \tag{8}$$

The following approximation is proposed for k_{emx}:

$$\frac{k_{emx}}{k_0} \cong \frac{k\{T_{mx}\}}{k\{T_0\}} = \frac{k_\infty e^{-E/RT_{mx}}}{k_\infty e^{-E/RT_0}} = e^{\frac{E}{RT_0}\left(1-\frac{T_0}{T_{mx}}\right)} \tag{9}$$

Eq. (9) 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.

In order 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:

$$u_m\pi a^2(T_{mx}-T_0)c\rho = C_{A0}\,Z_{mx}\,q_M\,u_m\pi a^2 x + 2\pi a x j_w \tag{10}$$

Eq. (10) can be re-arranged and re-expressed in the following form:

$$\frac{T_{mx}}{T_0} = 1+\frac{C_{A0}Z_{mx}q_M x}{\rho c u_m T_0}+\frac{2j_w x}{a u_m \rho c T_0} = 1+Z_{mx}\tau+\left(\frac{4K_{x0}}{\mathrm{Re}\mathrm{Pr}K_{a0}}\right)J \tag{11}$$

The second and third terms on the right-hand side of Eq. (11) represent the contributions of reaction and heat exchange, respectively, to the mixed-mean temperature.

Eq. (8) constitutes the basic analogy between reaction and heat transfer, but Eqs. (9) and (11) are needed for its implementation. These three equations can be combined to obtain the following expanded expression of the analogy:

$$Nu_x = \frac{Nu_{ox}}{1+\beta\xi\left(1-Z_{mx}\right)\exp\left\{\dfrac{E/RT_0}{1+\left(\tau\left[Z_{mx}+\left(K_{x0}/\xi\right)\right]\right)^{-1}}\right\}} \tag{12}$$

Eq. (12) provides a relationship between the local Nusselt number and the local mixed-mean conversion. It incorporates a number of fixed parameters and one arbitrary coefficient,

namely β. That coefficient is the counterpart of the arbitrary coefficients and exponents of the classical analogies between momentum and heat transfer. Eq. (12) includes implicit idealizations in structure just as do the classical analogies. In this case the implicit idealizations are those of Eqs. (4) and (9). The 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. (11), thereby allowing the formulation of a direct relationship between Nu_x and Z_{mx}, namely Eq. (12). 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. (8) remains valid if J_x is simply substituted for J, that is, if ξ is replaced by $\xi_x \equiv \tau RePrK_{a0}/4J_x$. For a uniform wall-temperature, the expanded form of the analogy is thus

$$Nu_x = \frac{Nu_{oxT}}{1+\beta\xi_x(1-Z_{mx})\exp\left\{\frac{E}{RT_0}\left(1-\frac{T_0}{T_{mx}}\right)\right\}} \tag{13}$$

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, namely

$$Nu_x = \frac{2aj_w}{\lambda(T_w - T_m)} = \frac{2J_x}{\frac{T_w}{T_0} - \frac{T_{mx}}{T_0}} \tag{14}$$

It follows from Eq. (14) that

$$\xi_x = \frac{\tau\ \mathrm{Re}\ \mathrm{Pr}\ K_{a0}}{2\,Nu_x\left(\frac{T_w}{T_0} - \frac{T_{mx}}{T_0}\right)} \equiv \frac{\zeta}{Nu_x\left(\frac{T_w}{T_0} - \frac{T_{mx}}{T_0}\right)} \tag{15}$$

Here $\zeta \equiv \tau RePrK_{a0}/2$ is the characteristic group of specified variables for a uniform wall-temperature. Substituting for ξ_x from Eq. (15) in Eq. (11), followed by rearrangement, results in the following expression explicit in Nu_x:

$$Nu_x = Nu_{oxT} - \left(\frac{\beta\zeta(1-Z_{mx})}{\frac{T_w}{T_0} - \frac{T_{mx}}{T_0}}\right)\exp\left\{\frac{E}{RT_0}\left(1-\frac{T_0}{T_{mx}}\right)\right\} \tag{16}$$

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

Eqs. (13) and (16) 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. (12). Even so, they

have possible value in predicting the effect of the various parameters that are encompassed. Eq. (16) has a small advantage over Eq. (13) 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 only of the Reynolds number. On the other hand, the mixed–mean conversion is a function of the dimensionless distance through the tube, of the dimensionless rate of heat exchange with the wall, and of all of the dimensionless variables and parameters that determine the rate of reaction. This complex dependence might appear to preclude the derivation of an algebraic expression for Z_{mx} as function of τ and J, but Churchill and Yu [5] devised a set of empirical expressions that can be consolidated to the following approximate one:

$$Z_{mx} = \frac{1-e^{-0.96K_{0x}}}{1-3.85\tau} + \frac{250JK_{0x}}{\mathrm{Re}} \tag{17}$$

Eq. (17) provides reasonable predictions for uniform heating for all conditions. Churchill and Yu[9] also devised an empirical expression for the prediction of Z_{mx} for uniform wall–temperature. but it is not reproduced here because Eqs. (13) and (16) are not proposed for quantitative predictions

The coefficient β in the proposed analogy for chemical reaction and heat transfer is the counterpart of γ in the Churchill-Zajic modification of the analogy of Reichardt. The latter quantity 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 dependence 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, but the independence of β from Q was encouraging and led to the speculative formulation of Eq. (3) and its detailed implementation in terms of Eqs. (12), (13), and (16). 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[6,7], who solved the partial differential equations 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. Since the focus

herein is on the analogy, the computed values of Z_{mx} by Yu and Churchill[7,8] 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. (12). The so-computed values of β at the arbitrary but representative value of $K_{x0} = 0.50$ are illustrated in Table1 for the 8 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 = 300K. 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 1 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 greater than 25 for one set of conditions (τ = 0.05 and J = −0.05) and by a factor of greater than 4 for the converse condition (τ = −0.05 and J = 0.05). In this respect, Eq. (12) compares favorably with the analogy of Reichardt as improved by Churchill and Zajic[7]. However, the coefficient γ in the improved analogy 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.

Table 1. Variance of Coefficient β in Laminar Flow at Re = 400 with Pr = 0.7, Sc = 0.2, $E/R/T_0$ = 17.815, T_0 = 300K and K_{x0} =0.50, for which Nu_{ox} = 6.2994

τ	J	$-\xi$	Z_{mx}	Nu_x	T_{mx}/T_0	k_{emx}/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

The dependence of β on K_{x0} is examined in Tables 2 and 3. 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 3, the combination of τ = −0.01 and 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[6] of the numerically computed values of β versus $ln\{K_{x0}\}$ for all eight of the test conditions suggested the following empirical correlating equation:

$$\beta = A + B \ln\{K_{x0}\} \tag{18}$$

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

Table 2. Selected Characteristics for Uniform Heating in Fully Developed Laminar Flow at Re = 400 with Pr = 0.7, Sc = 0.2, K_{a0} = 0.096, τ = –0.01, J = 0.05, and ξ = –1.344

K_{0x}	Z_{mx}	Nu_{xo}	Nu_x	T_{mx}/T_0	k_{emx}/k_0	- Q_x	β	B_{19}
0.01	0.009853	22.135	24.844	0.99998	0.9995	1.330	0.0820	0.0453
0.02	0.019588	17.523	20.212	0.99995	0.9992	1.317	0.1013	0.0789
0.05	0.048104	12.893	15.487	0.99989	0.9981	1.290	0.1309	0.1238
0.10	0.09347	10.268	12.685	0.99981	0.9966	1.214	0.1569	0.1569
0.20	0.17713	8.239	10.360	0.99971	0.9948	1.100	0.1860	0.1905
0.50	0.38281	6.299	7.8202	0.99988	0.9981	0.828	0.2349	0.2349
1.00	0.61921	5.306	6.2691	1.00121	1.0225	0.523	0.2937	0.2685
2.00	0.86258	4.687	5.1198	1.00618	1.1171	0.206	0.4096	0.3021

$$\beta = 0.2585 + 0.04846\ ln\{K_{x0}\} \tag{19}$$

The representation of β by Eq. (19) is seen in Table 2 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. (19) would result in different values of A and B but would not change the overall accuracy of the predictions of β and Nu_x significantly.

Table 3. Selected Characteristics for Uniform Heating in Fully Developed Laminar Flow at Re =400 with Pr = 0.7, Sc = 0.2, K_{a0} = 0.096, τ = 0.05, J = −0.05, and ξ = −6.7

K_{x0}	Z_{mx}	Nu_{xo}	Nu_x	T_{mx}/T_0	k_{emx}/k_0	$-Q_x$	β	β_{20}	Nu_{x20}
0.01	0.009858	22.135	46.4443	1.000421	1.00752	6.703	0.07809	0.07809	38.74
0.02	0.01965	17.523	48.5847	1.000834	1.01495	6.686	0.09562	0.88075	42.62
0.03	0.02940	15.291	53.5328	1.001247	1.02243	6.669	0.10712	0.10219	48.01
0.04	0.03910	13.888	59.5900	1.001657	1.02991	6.650	0.11533	0,11220	54.70
0.05	0.04875	12.893	67.7090	1.002066	1.03741	6.631	0.12209	0.11997	63.05
0.06	0.05836	12.137	78.0892	1.002472	1.04491	6.612	0.12773	0.12631	73.64
0.07	0.06793	11.536	91.5932	1.002876	1.05241	6.592	0.13259	0.13168	87.40
0.08	0.07745	11.041	109.7004	1.003278	1.05993	6.571	0.13687	0.13632	105.9
0.09	0.08694	10.625	135.0736	1.003677	1.06745	6.550	0.14066	0.14042	132.4
0.10	0.09635	10.268	172.8324	1.004073	1.07495	6.528	0.14409	0.14409	172.9
0.20	0.18821	8.239	169.1569	1.007922	1.15031	6.275	0.15160	0.16821	148.3
0.30	0.27508	7.286	92.1840	1.011522	1.22498	5.967	0.15434	0.18233	82.85
0.40	0.35635	6.702	94.6500	1.014841	1.29762	5.613	0.16554	0.19234	84.20
0.50	0.43155	6.299	161.3508	1.017857	1.36690	5.222	0.18402	0.20010	140.16
0.60	0.50041	6.001	770.5875	1.020556	1.43165	4.806	0.20645	0.20645	759.2
0.70	0.56283	5.769	90.2592	1.022933	1.49093	4.380	0.21372	0.21182	79.85
0.80	0.61893	5.584	44.6118	1.024994	1.54405	3.954	0.22125	0.21646	38.75
0.90	0.66893	5.432	28.8255	1.027750	1.61772	3.599	0.22549	0.22056	26.35
1.00	0.71317	5.306	21.0948	1.028218	1.63053	3.143	0.23814	0.22423	17.97
2.00	0.93597	4.687	6.6234	1.031918	1.73503	0.747	0.39134	0.24835	5.76

As Illustrated in Table 3, 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. (18) at the two peak values in Nu_x, that is at $K_{x0} = 0.10$ and 0.60, results in

$$\beta = 0.2242 + 0.03480\ ln\{K_{x0}\} \tag{20}$$

The predictions of β by Eq. (20) are again somewhat crude and the corresponding ones of Nu_x represent the chaotic behavior only semi-quantitatively, 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. (19) and (20) 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 4 illustrates the variance of β at $K_{x0} = 0.5$ for turbulent flow at Re = 37,640, but otherwise the same 8 conditions as for Table 1. The results, however, differ greatly. 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 variance and an explanation for the differences relative to Table 1, finite-difference computations were carried out by Yu and Churchill[6] for 16 additional conditions, primarily involving greater absolute values of the dimensionless heat flux density J, but herein attention is confined to the conditions of Table 6. As can be deduced from Eq. (7), the negative values of β correspond t from the attenuation of Nu_x relative to Nu_{ox}. The difference in the values of β in Tables 1 and 4 indicates that the dependence on Re is not wholly characterized by it's presence in ξ, at least insofar as one condition is in the laminar regime and the other in 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 $(k_{emx}/k_0)(1-Z_{mx})$.

Table 4. Variance of Coefficient β at $K_{x0} = 0.50$ in Turbulent Flow at Re = 37,640 with Sc = 0.2, $E/R/T_0$ = 17.815, T_0 = 300K and Pr = 0.7,for which Nu_{ox} = 107.69

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

Tables 5 and 6, which illustrate the dependence of Nu_x, β, and other dependent variables on K_{x0} and which include Nu_{ox} as a reference, constitute a counterpart to Tables 2 and 3. In the turbulent regime, Nu_{ox} depends separately on Re, Pr, and a/x rather than on Gz

$= \pi RePra/x$ only. Hence 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 non-monotonic dependence of β on K_{x0}.

Table 5. Selected Characteristics for Uniform Heating in Fully Developed Turbulent Flow at Re = 37640 with Pr = 0.7, Sc = 0.2, K_{a0} = 0.096, τ = −0.01, J = 0.05, and ξ = −126.47

K_{x0}	Z_{mx}	Nu_{xo}	Nu_x	T_{mx}/T_0	k_{emx}/k_0	$-Q_x$	β	β_{22}	Nu_{x22}
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

Table 6. Selected Characteristics for Uniform Cooling in Fully Developed Turbulent Flow **at** Re= 37640 with Pr = 0.7, Sc = 0.2, K_{a0} = 0.096, τ = 0.05, J = −0.05, and ξ = −632.3

K_{x0}	Z_{mx}	Nu_{xo}	Nu_x	T_m/T_0	k_{emx}/k_0	$-Q_x$	$-\beta$	$-\beta_{23}$	Nu_{x23}	$-\beta_{24}$	Nu_{x24}
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

The behavior for τ = -0.01 and J = 0.05 is summarized in Table 5. Since β goes through a minimum as K_{x0} increases, Eq. (18) is obviously inadequate, and the following expression is proposed as an alternative:

$$\beta = A + B\left(\ln\{K_{x0}\} - \frac{K_{x0}}{K_{x0c}} \right) + C\left(\ln\left\{ \frac{K_{x0}}{K_{x0c}} \right\} \right)^2 \tag{21}$$

Eq. (21) was formulated to result in $d\beta/dK_{x0} = 0$ at $K_{x0} = K_{x0c}$, that 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 semi-logarithmic dependence. 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

$$\beta = -0.01971 - 0.009201\left(\ln\{K_{x0}\} - \frac{K_{x0}}{0.20} \right) - 0.001795\left(\ln\left\{ \frac{K_{x0}}{0.20} \right\} \right)^2 \tag{22}$$

The accuracy of the predictions of β by Eq. (22) is seen in Table 5 to be only fair, but the resulting predictions of Nu_x are perhaps, in consideration of the erratic behavior, of acceptable accuracy.

For $\tau = 0.05$ and $J = -0.05$, as shown in Table 6, 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:

$$-\beta = 0.01739 + 0.02919\ ln\{K_{x0}\} \tag{23}$$

The corresponding values of Nu_x in that range of K_{0x} are seen to be of acceptable accuracy. On the other hand the values of β for $0.6 \leq K_{0x} \leq 1.0$ 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:

$$-\beta = 0.1519 + 0.09\left(\ln\{K_{x0}\} - \frac{K_{x0}}{0.60} \right) + 0.04482\left(\ln\left\{ \frac{K_{x0}}{0.60} \right\} \right)^2 \tag{24}$$

The predictions of Nu_x by Eq. (24), including the peak value, are seen to be 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. (23) and (24) 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. (16) using the values of Nu_x, Z_{mx}, and T_{mx}/T_0 computed by Yu and Churchill[7]. Values for $K_{x0} = 0.50$ are listed in Table 7 for a laminar flow and in Table 8 for a turbulent flow. The values of β for 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 enhanced greatly 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. The computed values of β vary monotonically with K_{x0} and the behavior in each case could be represented by Eq. (18) but this was not done because a supplementary correlation for T_{mx}/T_0 would be required to predict Nu_x.

Table 7. Variance of β at $K_{x0} = 0.50$ with τ and T_w/T_0 Laminar Flow at $Re = 400$ with $Pr = 0.7$, $Sc = 0.2$, $E/R/T_0 = 17.815$, $T_0 = 300$K for which $Nu_{ox} = 5.0383$,

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

Table 8. 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, $E/R/T_0$ = 17.815, and T_0 = 300K

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

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 focussed on these unresolved issues in two categories. First, the proposed analogy is compared with the classical ones for momentum and heat transfer. Second, the utility of the new analogy is examined *vis-à-vis* the finite-difference solution of the partial differential equations of conservation.

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

The classical analogies for momentum and heat transfer 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.

The new analogy resembles the classical ones superficially 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, the classical analogies relate the transport of two different quantities, momentum and energy, whereas the new one 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 in the new one. Moreover, the classical analogies relate two fully developed processes whereas the new analogy relates two developing processes. The classical analogies apply only for turbulent flow while the new analogy is applicable for both laminar and turbulent flow. 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 previous paragraph, the derivation of the new analogy followed a completely different procedure than that utilized for any of the classical ones. First, an exact solution for heat transfer was derived for a very, very 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, namely 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. Hence, 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, because 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[8] in series form are a function only of $wc/\lambda x = (\pi a/2x)RePr$ 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 48/11of 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, an effective energy of activation, an overall heat of reaction, and a mean molecular weight, could be utilized to approximate the net effect of multiple reactions on the Nusselt number.

In summary, the new analogy differs fundamentally from the classical ones in that it links two dissimilar processes, and has a much broader scope, encompassing developing as well as fully developed convection and reaction in both laminar and turbulent flow. The price of that difference and of the broader scope is a dependence of the coefficient β on many variables as compared to the dependence of γ in the modified analogy of Reichardt on the Reynolds number and mode of heating alone. Whereas the latter 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 2, 3, 4, and 6, limited to one case at a time.

An Explanation for the Enhancement and Attenuation

The analogy in the generic form of Eq. (4), as well as in the detailed form of Eqs. (12) and (16), 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 a serendipitous result of the independent variations of Q_x and β. However, this does not constitute a physical explanation. Although Eq. (5) provides essentially exact values of Q_x in terms of the specified variables, the dependence 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 on the velocity distribution, as well as 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[7] for uniform heating with and without reaction confirm this conjecture for both laminar and turbulent flow.

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 due to a reaction that were identified are those Edwards and Ferguson[9] 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. (12), 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, as for example, those that make up Eqs. (12) and (16). Although the indicated functional dependence of Nu_x on these several dimensionless groupings may not be exact because of the speculations and approximations utilized 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. (12) and (16) 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 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 dependence 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 ones between momentum and heat transfer.

The new analogy has a broader scope than the classical ones 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. Progress in this respect is currently limited to the observation of a limited variance for different thermal conditions and a nearly semi-logarithmic dependence on distance through the reactor/exchanger.

Although the derivation herein is based on a single, irreversible, equimolar reaction the new analogy 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 postulate of plug flow, which is made in many books on reaction engineering, precludes the formulation of an analogy as well as the calculation of the enhancement and attenuation of the heat transfer coefficient that it explains.

References

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1. Reichardt, H. (1951), "Die Grundlagen des turbulenten Wärmeüberganges" *Arch. Ges. Wärmetechn* **2**,129–142..
2. Churchill, S.W. (1997), "Critique of the classical algebraic analogies between heat, mass, and momentum transfer", *Ind. Eng. Chem. Res.* **36**,3866–3878.
3. Churchill, S.W., and S.C. Zajic (2002), " Prediction of fully developed convection with minimal explicit empiricism", *AIChE J.* **48,** 927-940.
4. Churchill, S.W. (2005), "Interaction of chemical reactions and transport. 1. An overview", *Ind. Eng. Chem. Res.* **44**,5199–5212.
5. Churchill, S.W., and YU Bo (2005), "The effects of transport on reactions in homogeneous tubular flow', Preprint, CD-ROM, AIChE Annual Meeting, AIChE, NY, NY; full version, *Ind. Eng. Chem. Res*. in press.
6. YU Bo and S.W. Churchill, "Effects of energetic reactions on forced convection in a round tube with a uniform heat flux density on the wall". In review.

7. YU Bo and S.W. Churchill, ". Effects of energetic reactions on forced convection in a round tube with a uniform temperature on the wall. In review.
8. Graetz L. (1883), "Über die Wärmeleitungsfahigkeit von Flüssigkeiten", *Ann. Phys. Chem.* **18**, 79–94..
9. Edwards, L. L., and R.R Furgason (1968), "Heat Transfer in Thermally Decomposing Ozone", *Ind. Eng. Chem. Fundam.* **7**, 441-445.