



Laminar free convection from a vertical plate in partly dissociated gases

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Abstract

Two-dimensional steady free convection from an isothermal vertical plate is studied in a gas where a reversible very fast reaction of dissociation $A \leftrightarrow 2B$ takes place at atmospheric pressure. The effective properties in the presence of dissociation are evaluated. The governing boundary-layer equations are solved numerically for a wide range of values of the independent variables. All the data obtained are correlated by a single correlation even if the temperature interval in the boundary layer (T_W , T_∞) is allowed to vary in a wide range, both in relative location and width, in respect to the temperature interval of dissociation. The correlated dimensionless parameters include the ratio ρ_W/ρ_∞ and are defined through the mixture effective properties calculated at T_W and T_∞ . The maximum absolute value of the relative error results to be dependent essentially by two particular parameters related to the variations of α and ρ^* in the boundary layer. © 2000 Elsevier Science Ltd. All rights reserved.

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1. Introduction

In systems where a chemical reaction of dissociation–recombination takes place, the total heat transfer may be increased owing to the energy transfer by diffusion due to a concentration gradient. Most of the previous work on this subject has been developed in the fields of combustion [1–9], rocket propulsion [10–13], hypersonic flows and re-entry problems [1,14–17], essentially with reference to forced convection [1–17]. Free convection has been studied for laminar flames [5–8], but without taking into account dissociation effects. Most of the works dealing with dissociation [1,4,5,8,10–13,15,16] hypothesizes that the chemical system is one in which the migration to

products is very fast compared to the rates of diffusion and convection through the boundary layer; assuming in fact the existence of complete chemical equilibrium. Other works [2,3,7,9,14] take into account finite chemical reaction times.

In the presence of dissociation, the total heat transfer by forced convection may be increased essentially owing to the energy of dissociation–recombination transferred by diffusion.

On the other hand, since dissociation greatly affects gas density and thus the related buoyancy forces, in free convection it has a direct influence on both the transfer properties and the flow driving forces. This phenomenology seems much less investigated.

It is the purpose of the present paper to analyze free convection heat transfer in a dissociating gas, assuming very fast migration to products of complete chemical equilibrium.

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Nomenclature

A, B	chemical species	Pr	Prandtl number
C_p	specific heat at constant pressure	Gr	Grashof number
D	coefficient of diffusion		
g	gravitational constant	<i>Greek symbols</i>	
h	local heat transfer coefficient	α	fraction of moles of A dissociated
\bar{h}	average heat transfer coefficient	λ	thermal conductivity
H	specific enthalpy	μ	dynamic viscosity
J	specific flux of matter with respect to mass average velocity	$\tilde{\chi}$	mole fraction
K	equilibrium constant	ρ	mass density
L	height of the wall	$\tilde{\rho}$	molar density
M	molecular weight		
P	pressure	<i>Subscripts</i>	
q	specific heat flux	i, j	referred to species A and B
R_0	constant of gases	FR	referred to the frozen mixture
T	absolute temperature	X	in the X direction
$T_{0.5}; T_{0.99}$ etc.	temperature related to the value of $\alpha = 0.5$ or $\alpha = 0.99$ etc.	ref	reference
u	axial velocity component	T_{ref}	at the reference temperature
v	normal velocity component	T	at temperature T
x	longitudinal coordinate	∞	far from the wall surface
y	normal coordinate		
ΔH	heat of dissociation	<i>Superscript</i>	
$\Delta T_{0.99}$	$= T_{0.995} - T_{0.005}$	*	referred to the reacting system ('effective' property)
Nu	Nusselt number		

2. Case of interest and theoretical hypotheses

Two-dimensional steady free convection from an isothermal vertical plate at a temperature T_W is studied in a gas where a reversible very fast reaction of dissociation $A \leftrightarrow 2B$ takes place at atmospheric pressure. Both A and B are treated as perfect gases with constant properties except density. Laminar boundary-layer flow is assumed. Viscous dissipation, work against gravity field and thermal diffusion are neglected. The fluid temperature T_∞ outside the boundary layer and the pressure P throughout the boundary layer are assumed uniform. The existence of chemical equilibrium at any point in the system is assumed.

3. Effective properties

3.1. Viscosity μ^*

In the presence of dissociation, the mixture viscosity is evaluated as for a 'frozen' (non reacting) mixture of perfect gases through the Wilke's relations [18]:

$$\mu^* = \mu_{FR} = \frac{\sum_i \mu_i \tilde{\chi}_i}{\sum_j \tilde{\chi}_j \phi_{ij}},$$

$$\phi_{ij} = \frac{\left[1 + \left(\frac{\mu_i}{\mu_j} \right)^{1/2} \left(\frac{M_j}{M_i} \right)^{1/4} \right]^2}{\left[8 \left(1 + \frac{M_i}{M_j} \right) \right]^{1/2}}$$

$(i = A, B \text{ and } j = A, B)$

where μ_i (or μ_j), $\tilde{\chi}_i$ (or $\tilde{\chi}_j$) and M_i (or M_j) are, respectively, the viscosity, the mole fraction and the molecular weight of the i th (j th) component of the mixture.

3.2. Conductivity λ^*

By introducing a 'frozen' conductivity of the mixture, still defined according to Wilke:

$$\lambda_{FR} = \frac{\sum_i \lambda_i \tilde{\chi}_i}{\sum_j \tilde{\chi}_j \phi_{ij}} \quad (i = A, B \text{ and } j = A, B) \quad (2)$$

where λ_i is the thermal conductivity of the i th component of the mixture, the total heat flux q_x at a distance x from the leading edge of the plate is obtained by the sum of the contributions due to the thermal conduction and the diffusion–recombination:

$$q_x = -\lambda_{FR} \frac{\partial T}{\partial y} + J_B \Delta H, \tag{3}$$

where $\partial T/\partial y$ is the local value of the temperature gradient normal to the plate, J_B is the specific mass flow of B and ΔH is the heat of dissociation.

Since the type of diffusion involved is neither equimolar nor diffusion through a stagnant film, J_B may be expressed through the general form of Fick’s law [13]:

$$J_B = -M_B D_{BA} \tilde{\rho}_A \frac{1}{1 - \alpha} \frac{\partial \alpha}{\partial y} = -M_B D_{BA} \frac{\rho_A}{M_A} \frac{1}{1 - \alpha} \frac{\partial \alpha}{\partial y}, \tag{4}$$

where D_{BA} is the coefficient of diffusion of B through A, $\tilde{\rho}_A$ is the molar density of A, α is the fraction of

$$\alpha = \frac{\frac{\alpha_{ref}^2}{1 - \alpha_{ref}^2} \exp\left(\frac{M_A}{R_0} \left\{ [\Delta H_{T_{ref}} - (C_{pB} - C_{pA}) T_{ref}] \left(\frac{1}{T_{ref}} - \frac{1}{T} \right) + (C_{pB} - C_{pA}) \ln \frac{T}{T_{ref}} \right\} \right)}{1 - \frac{\alpha_{ref}^2}{1 - \alpha_{ref}^2} \exp\left(\frac{M_A}{R_0} \left\{ [\Delta H_{T_{ref}} - (C_{pB} - C_{pA}) T_{ref}] \left(\frac{1}{T_{ref}} - \frac{1}{T} \right) + (C_{pB} - C_{pA}) \ln \frac{T}{T_{ref}} \right\} \right)}. \tag{9}$$

dissociated moles of A and ρ_A is the density of gas A undissociated at the given temperature and pressure. Since $M_B/M_A = 1/2$, it results:

$$J_B = -D_{BA} \rho_A \frac{1}{1 - \alpha} \frac{\partial \alpha}{\partial y} \tag{5}$$

Under the assumption of chemical equilibrium, α is a function of the only temperature, thus resulting $\frac{\partial \alpha}{\partial y} = \frac{d\alpha}{dT} \frac{\partial T}{\partial y}$, and we may then define the ‘effective’ conductivity:

$$\lambda^* = -\left(\lambda_{FR} + D_{BA} \rho_A \Delta H \frac{1}{1 - \alpha} \frac{d\alpha}{dT} \right). \tag{6}$$

The expressions of α and $\partial \alpha/\partial T$ to be introduced in Eq. (6) may be evaluated by using the van’t Hoff equation

$$\frac{d(\ln K_p)}{dT} = \frac{M_A \Delta H}{R_0 T^2}, \tag{7}$$

with

$$K_p = \frac{4\alpha^2}{1 - \alpha^2} \frac{P}{P_{ref}}$$

and $\Delta H = \Delta H(T)$

$$= \Delta H(T_{ref}) + (C_{pB} - C_{pA})(T - T_{ref}),$$

where P_{ref} and T_{ref} are the reference pressure and temperature. C_{pA} and C_{pB} are the specific heats at constant pressure for A and B.

Being $P = P_{ref}$;

$$\alpha(T_{ref}) = \alpha_{ref} = \sqrt{\frac{K_{p_{ref}}}{K_{p_{ref}} + 4}}$$

it then follows:

$$\frac{d\alpha}{dT} = \frac{[\Delta H(T_{ref}) + (C_{pB} - C_{pA})(T - T_{ref})] M_A}{2R_0 T^2} \alpha(1 - \alpha^2) \tag{8}$$

and

3.3. Density ρ^*

From the state equation for perfect gases, it follows:

$$\rho^* = \frac{P_{tot} M_A}{R_0 (1 + \alpha) T}. \tag{10}$$

3.4. Specific heat at constant pressure C_p^*

From the enthalpy of the mixture:

$$H = (1 - \alpha) C_{pA} (T - T_{ref}) + \alpha [C_{pB} (T - T_{ref}) + \Delta H] \tag{11}$$

it follows:

$$C_p^* = \frac{dH}{dT} = [(1 - \alpha) C_{pA} + \alpha C_{pB}] + \Delta H \frac{d\alpha}{dT}. \tag{12}$$

Since P is assumed constant within the boundary layer, the effective properties discussed above are functions of the only temperature. Fig. 1 shows the typical distributions of α and both the effective and ‘frozen’ properties with temperature, where the subscript of temperature denotes the percent of dissociation. It may be noticed that:

- λ^* and C_p^* undergo large variations with temperature up to ten times the frozen values, with a maximum for $\alpha \cong 0.5$;
- λ^* and C_p^* have similar distributions, so that the variations of the effective Prandtl number Pr^* with temperature are smaller than those pertinent to λ^* and C_p^* ;
- the variation of ρ^* with temperature is much larger than those pertinent to ρ_A and ρ_B .

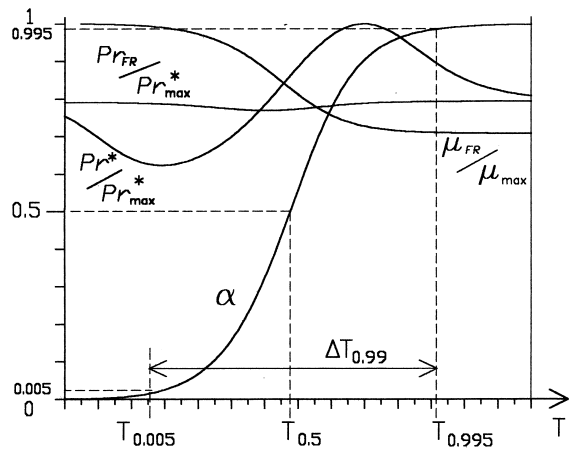
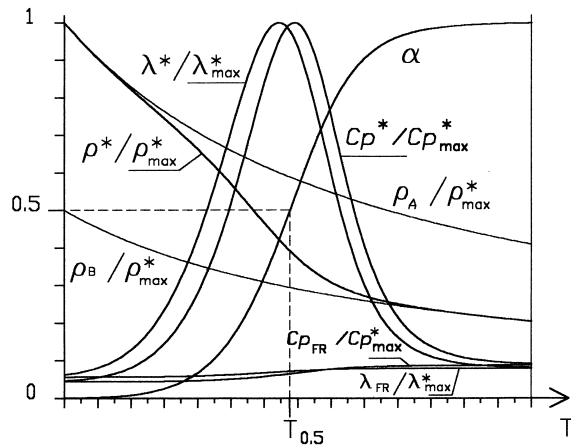


Fig. 1. Variation of the effective properties with temperature in the interval of dissociation.

4. Governing equations

The equations of continuity, mean motion and energy are expressed in the following ξ, ω coordinate system (Fig. 2):

$$\xi = x \quad \omega = y/\Psi(x), \tag{13}$$

where $\Psi(x) = C_1 x^\beta$, with C_1 and β constants

Continuity

$$\frac{\partial \rho^* u}{\partial \xi} + \frac{1}{\Psi} \frac{\partial \rho^* v}{\partial \omega} - \frac{\omega}{\Psi} \frac{d\Psi}{dx} \frac{\partial \rho^* u}{\partial \omega} = 0 \tag{14}$$

Momentum (mean mass flow)

$$\rho^* u \frac{\partial u}{\partial \xi} + \left(\frac{\rho^* v}{\Psi} - \rho^* u \frac{\omega}{\Psi} \frac{d\Psi}{dx} \right) \frac{\partial u}{\partial \omega} - \frac{1}{\Psi^2} \frac{\partial}{\partial \omega} \left(\mu_{FR} \frac{\partial u}{\partial \omega} \right) + g(\rho^* - \rho_\infty^*) = 0, \tag{15}$$

which, taking into account Eq. (14), becomes:

$$\frac{\partial}{\partial \xi} (\rho^* u \Psi u) + \frac{\partial}{\partial \omega} \left[u \left(\rho^* v - \rho^* u \omega \frac{d\Psi}{dx} \right) - \frac{\mu_{FR}}{\Psi} \frac{\partial u}{\partial \omega} \right] + g(\rho^* - \rho_\infty^*) = 0 \tag{16}$$

Energy

$$\frac{\partial}{\partial \xi} (\rho^* u \Psi h) + \frac{\partial}{\partial \omega} \left[h \left(\rho^* v - \rho^* u \omega \frac{d\Psi}{dx} \right) - \frac{\lambda^*}{\Psi} \frac{\partial T}{\partial \omega} \right] = 0 \tag{17}$$

or

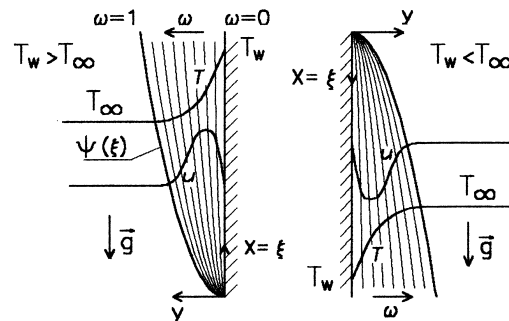


Fig. 2. Physical model coordinate system.

$$\frac{\partial}{\partial \xi} (\rho^* u \Psi C_p^* T) + \frac{\partial}{\partial \omega} \left[C_p^* T \left(\rho^* v - \rho^* u \omega \frac{d\Psi}{dx} \right) - \frac{\lambda^*}{\Psi} \frac{\partial T}{\partial \omega} \right] = 0 \quad (18)$$

Boundary conditions

$$\omega = 0; \quad \xi \geq 0: \quad u = v = 0; \quad T = T_W \quad (19)$$

$$\omega \rightarrow \infty; \quad \xi \geq 0:$$

$$u = v = 0; \quad \frac{\partial u}{\partial \omega} = \frac{\partial v}{\partial \omega} = 0; \quad T = T_\infty; \quad \frac{\partial T}{\partial \omega} = 0$$

5. Method of solution

The set of equations (Eqs. (14) and (16)–(19)) has been solved by a finite-differences method with control volumes formulation and assuming ξ as one-way coordinate. In the derivation of the discretization equation, along the ξ direction the downstream values of the dependent variable are assumed to prevail over the entire $\Delta\xi$ of the control volume (fully implicit scheme), while along the ω direction the exponential scheme [19] has been considered.

The $\Delta\xi$ intervals have been assumed equal to or smaller than $\Psi(x)/4$. The values of C_1 and β in the $\Psi(x)$ expression reported in Eq. (13) have been assumed by a few trials so that the thermal and velocity boundary layers were contained in the interval $0 \leq \omega \leq 1$. The values pertinent to the case of a fluid with constant properties evaluated at $T = (T_W + T_\infty)/2$ have been assumed as first approximation values. The number of grid nodes in the ω coordinate has been chosen so that at least forty grid nodes were contained within the boundary layers. As far as the spacing along ω is concerned, uniform intervals $\Delta\omega$ and $2\Delta\omega$ have been assumed respectively for $0 \leq \omega \leq 0.7$ and $0.7 \leq \omega \leq 1$.

For each spatial interval in the ξ direction, both smallness of values and flatness of T and u profiles have been verified through:

$$|T_M - T_\infty| \leq |T_W - T_\infty| \times 10^{-3}; \quad u_M \leq u_{\max} \times 10^{-3}$$

$$|T_M - T_{M-1}| \leq |T_W - T_\infty| \times 10^{-4};$$

$$|u_M - u_{M-1}| \leq u_{\max} \times 10^{-4}$$

Owing to the strong non-linearities essentially due to the effect of the temperature on dissociation and then on the fluid properties, within each discretization step along the ξ direction iterations have been performed

on the temperature and velocity fields until convergence.

6. Numerical experiments and heat transfer analysis

The thermal and velocity fields have been solved for a wide range of values of the independent variables which have influence on the effects pertinent to dissociation:

$$2.8 \times 10^{-6} \leq D_{BA} \leq 2.5 \times 10^{-5} \quad (\text{m}^2/\text{s})$$

$$200 \leq \Delta H(T_{\text{ref}}) \leq 1900 \quad (\text{kJ/kg})$$

$$220 \leq T_{0.5} \leq 1400 \quad (\text{K})$$

$$2 \times 10^{-23} \leq K_p(T_{\text{ref}} = 298 \text{ K}) \leq 4 \times 10^8 \quad (\text{dimensionless})$$

$$T_{0.5} - 3\Delta T_{0.99} \leq T_W, \quad T_\infty \leq T_{0.5} + 3\Delta T_{0.99} \quad (\text{K})$$

thus resulting:

$$4 \times 10^{-3} \leq \rho^* \leq 9 \quad (\text{kg/m}^3)$$

$$361 \leq C_p^* \leq 109\,000 \quad (\text{J/kg/K})$$

$$9.2 \times 10^{-3} \leq \lambda^* \leq 3.2 \quad (\text{W/m/K})$$

$$1.3 \times 10^{-5} \leq \mu^* = \mu_{\text{FR}} \leq 2.1 \times 10^{-5} \quad (\text{Pa s})$$

$$0.5 \leq |T_W - T_\infty| \leq 1420 \quad (\text{K})$$

$$0.18 \leq Pr^* \leq 4.4 \quad (\text{dimensionless})$$

Two kinds of gases are studied:

A, biatomic, $M_A = 32$ and B, monoatomic, $M_B = 16$ (as for $\text{O}_2 \leftrightarrow 2\text{O}$)

A, polyatomic, $M_A = 92$ and B, polyatomic, $M_B = 46$ (as for $\text{N}_2\text{O}_4 \leftrightarrow 2\text{NO}_2$)

The pertinent values of C_p have been assumed as for perfect gases; the values of λ and μ for the dissociated species have been assumed from the undissociated values as proportional to $M^{1/2}$ [18]. The cases studied have been grouped in seven values of the effective Grashof number Gr^* in the range $5 \times 10^5 \div 1.8 \times 10^9$. For each gas the following computational procedure has been developed:

- select randomly a value of D_{BA} , $\Delta H(T_{\text{ref}})$, $T_{0.5}$, T_W and T_∞ in the appropriate ranges and derive the related value of K_p ;

- calculate the value of the height of the wall L pertinent to the given value of Gr^* (for all the cases studied it has resulted: $0.05 \text{ m} \leq L \leq 12 \text{ m}$);
- solve the governing equations.

For each value of Gr^* , 410 different cases have been solved. The random selection of both T_W and T_∞ in the above specified range $T_{0.5} - 3\Delta T_{0.99} \leq T_W$, $T_\infty \leq T_{0.5} + 3\Delta T_{0.99}$ has led with same probability to cases with $T_W > T_\infty$ and $T_W < T_\infty$.

The method of solution has been tested by solving 440 cases with both T_W and T_∞ well above or below the interval of dissociation so verifying the existence of the conditions required to the Boussinesq's approximation application.

The velocity and temperature fields have been solved and the local and total values h_x and \bar{h}_L of the convection heat transfer have been evaluated through:

$$h_x = \frac{q}{(T_W - T_\infty)} = -\lambda_w^* \left. \frac{\partial T}{\partial y} \right|_{y=0}, \tag{20}$$

where $\left. \frac{\partial T}{\partial y} \right|_{y=0}$ is calculated by a three-points interpolation, and:

$$\bar{h}_L = \frac{1}{L} \int_0^L h_x \, dx \tag{21}$$

Eqs. (1)–(12) have then allowed us to reduce the problem here analyzed to a free convection boundary layer flow and heat transfer with temperature-dependent properties.

For gases with $Pr = const$ and simple (like power-law) variations of λ , μ and C_p with temperature [20,21], the data obtained are successfully correlated by an equation:

$$Nu_\infty = Cost \, Gr_\infty^{m1} f(Pr) \Phi(T_W, T_\infty) \tag{22}$$

where $f(Pr)$ and $\Phi(T_W, T_\infty)$ are functions of the constants which figure in the power-law distributions assumed.

In the present case, the complexity of the dependence laws of the effective properties from temperature makes this method unsuitable. The gases here taken into account have instead some analogies with supercritical fluids [22], whose properties variations with temperature may be strong and non-monotonic. Correlations for supercritical fluids are usually expressed in the more traditional form:

$$Nu = Cost \, Gr^{m1} Pr^{m2} \tag{23}$$

where Nu , Gr and Pr are calculated with respect to the integrated mean property values or to the specially defined reference temperatures [22]. Nevertheless, in the present case the use of the integrated properties proved to be both unpractical and inaccurate.

In the present work, the best results were obtained by using the effective properties evaluated at T_W and T_∞ for the calculation of Nu , Pr and Gr and including the ratio ρ_W/ρ_∞ among the dimensionless parameters.

The most suitable correlation has proved to be:

$$\bar{Nu}_W = C \cdot Gr_\infty^{*m} Pr_\infty^{*n} \left(\frac{Pr_W^*}{Pr_\infty^*} \right)^p \left(\frac{\rho_W}{\rho_\infty} \right)^q \tag{24}$$

with

$$\bar{Nu}_W = \frac{\bar{h}_L L_{tot}}{\lambda_w^*}; \quad Gr_\infty^* = \frac{g|\rho_W^* - \rho_\infty^*| L^3 \rho_\infty^*}{\mu_{FRW}^2}; \tag{25}$$

$$Pr_W^* = \frac{C_{pW}^* \mu_{FRW}}{\lambda_w^*}; \quad Pr_\infty^* = \frac{C_{p\infty}^* \mu_{FR\infty}}{\lambda_\infty^*}.$$

The values of C , m , n , p , q have been calculated by the least-squares method through a logarithmic linear multiple regression. The validity of Eq. (23) has been tested both for the whole set of data and for several sub-sets of data related to different ranges of values of the independent variable. For all the tests carried out, the values of C , m , n , p , q obtained were essentially the same, but the scatter of data from Eq. (23) was higher for sets related to larger ranges of some variables (i.e.: $T_{0.5}$, T_W , T_∞ , $\Delta T_{0.99}$). Then, from the sensitivity analysis performed, the data scattering resulted mainly related to two parameters, $\Pi\alpha$ and $\Pi\rho$, defined as follows:

Parameter $\Pi\alpha$

$$\Pi\alpha = \hat{\alpha}_{max} / \hat{\alpha}_{min} \tag{26}$$

where $\hat{\alpha}_{max}$ and $\hat{\alpha}_{min}$ are the maximum and the minimum values of $\hat{\alpha}$ through the boundary layer, with $\hat{\alpha} = \alpha$ if $\alpha \leq 0.5$ and $\hat{\alpha} = 1 - \alpha$ if $\alpha > 0.5$; it then follows:

$$\hat{\alpha}_{min} = \min(\hat{\alpha}_W, \hat{\alpha}_\infty)$$

$$\hat{\alpha}_{max} = 0.5$$

$$\text{if } (\alpha_W \geq 0.5 \text{ and } \alpha_\infty \leq 0.5) \text{ or } (\alpha_W \leq 0.5 \text{ and } \alpha_\infty \geq 0.5)$$

$$\hat{\alpha}_{max} = \max(\hat{\alpha}_W, \hat{\alpha}_\infty)$$

$$\text{if } (\alpha_W \geq 0.5 \text{ and } \alpha_\infty \geq 0.5) \text{ or } (\alpha_W \leq 0.5 \text{ and } \alpha_\infty \leq 0.5)$$

Parameter $\Pi\rho$

$$\Pi\rho = \rho_W^* / \rho_\infty^* \quad \text{if } \rho_W^* > \rho_\infty^* \tag{27a}$$

$$\Pi\rho = \rho_\infty^* / \rho_W^* \quad \text{if } \rho_W^* \leq \rho_\infty^* \tag{27b}$$

The best fit of data has been obtained with the follow-

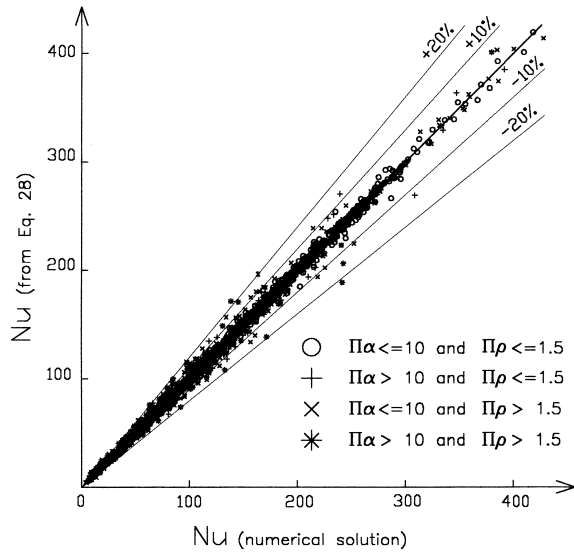


Fig. 3. Comparison between the Nusselt numbers predicted with Eq. (28) and the Nusselt numbers resulting from numerical experiments.

ing correlation (Fig. 3):

$$\bar{Nu}_W = 0.52 Gr_\infty^{*0.25} Pr_\infty^{*0.33} \left(\frac{Pr_W^*}{Pr_\infty^*} \right)^{0.55} \left(\frac{\rho_W}{\rho_\infty} \right)^{-0.2} \quad (28)$$

In Fig. 4 the standard deviation of data ε and the maximum absolute value of the relative error

$$|\eta| = \left| \frac{Nu_W(\text{Eq. (28)} - Nu_W(\text{datum}))}{Nu_W(\text{datum})} \right|$$

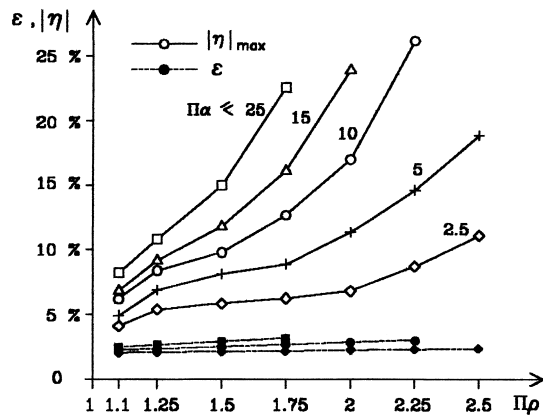


Fig. 4. Dependence of the standard deviation and the maximum absolute value of the relative error of the Nusselt numbers predicted with Eq. (28) on the $\Pi\alpha$ and $\Pi\rho$ parameters.

are reported against $\Pi\rho$ for different values of the maximum value of $\Pi\alpha$. It can be noticed that values of $|\eta|_{\max} < 10\%$ can be achieved for values of $\Pi\alpha < 10$ if a higher limit of 1.5 is wanted for $\Pi\rho$.

7. Conclusions

The heat transfer coefficients in two-dimensional free convection from an isothermal vertical plate in a gas where a reversible very rapid reaction of dissociation $A \leftrightarrow 2B$ takes place, may be expressed by a single correlation even if the temperature interval in the boundary layer (T_W, T_∞) is allowed to vary in a rather wide range, both in relative location and width, in respect to the temperature interval of dissociation. The correlated dimensionless parameters must include the ratio ρ_W/ρ_∞ and must be defined through the mixture effective properties calculated at T_W and T_∞ . The maximum absolute value of the relative error has resulted to be dependent essentially by two particular parameters related to the variations of α and ρ^* in the boundary layer.

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