

Dimensionless Numbers Expressed in Terms of Common CVD Process Parameters

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Abstract

A variety of dimensionless numbers related to momentum and heat transfer are useful in CVD analysis. These numbers are not traditionally calculated by directly using reactor operating parameters, such as temperature and pressure. In this paper, these numbers have been expressed in a form that explicitly shows their dependence upon the carrier gas, reactor geometry, and reactor operation conditions. These expressions were derived for both monatomic and diatomic gases using estimation techniques for viscosity, thermal conductivity, and heat capacity. Values calculated from these expressions compared well to previously published values. These expressions provide a relatively quick method for predicting changes in the flow patterns resulting from changes in the reactor operating conditions.

key words: dimensionless numbers, modeling, CVD, flow patterns

1. INTRODUCTION

Chemical vapor deposition (CVD) is an industrially important process involving both homogeneous and heterogeneous chemical reactions in which a solid film is deposited from the

gas phase onto a solid substrate. Since the often complex flow patterns inside a CVD reactor can greatly affect the purity and uniformity of the deposited film, it is important to be able to predict how they will change in response to changes in reactor conditions. While a complete computational model is required to provide detailed information regarding a process as complex as CVD, dimensionless numbers related to the flow can provide useful information on the relative magnitudes of various effects, such as how flow patterns vary with reactor operating conditions. These numbers are typically expressed in terms of viscosity, thermal conductivity, heat capacity, and density, as shown in Table 1. These common formulations do not readily show their dependence on common operating parameters, such as temperature and pressure.

Using estimation methods based on kinetic theory for viscosity, thermal conductivity, and heat capacity, expressions have been derived for some common dimensionless numbers useful in describing the flow in a CVD reactor: the Prandtl number (Pr), the Knudsen number (Kn), the Reynolds number (Re), thermal Peclet number (Pe), thermal Grashof number (Gr), and the thermal Rayleigh number (Ra). Each expressions is given in form:

$$\text{dimensionless number} = A \times B \times C \times D$$

where: A = a constant dependent on the units used for other parameters in the
expression

B = parameters related to the carrier gas used

C = parameters related to reactor geometry

D = parameters related to reactor operation conditions

Using these expressions, it should be possible to quickly determine the likely effects on the flow patterns of altering the reactor operation conditions. It is important to remember that the expressions for thermophysical properties and dimensionless numbers used in this paper are valid only when all variables are expressed in the units defined in this paper.

2. ESTIMATION OF THERMOPHYSICAL PROPERTIES

Since the chemically reacting species in CVD reactors are often present in very low concentrations, a dilute solution is assumed in this analysis so that the thermophysical properties of the gas in the reactor are those of the carrier gas. Ideal gas behavior is also assumed, which is a valid assumption at high temperatures and low pressures. CVD reactors typically operate at or below atmospheric pressures and at elevated deposition surface temperatures, thus satisfying the conditions for the ideal gas assumption.

The Chapman-Enskog theory may be employed to estimate the Newtonian viscosity if it can be validly assumed that: 1) the system is comprised of a dilute gas where only binary and elastic collisions occur; 2) the collisions are described by classical mechanics; and 3) the intermolecular potential is spherically symmetric [2]. These assumptions apply to low pressure, high temperature monatomic gases, but have also been found to be quite good for polyatomic gases [1]. From this theory, Newtonian viscosity may be expressed as:[2]

$$\mu = (2.669 \times 10^{-6}) \frac{(MT)^{0.5}}{\sigma^2 \Omega_{\mu}} \quad (1)$$

where: μ = Newtonian viscosity (kg/m-s)

M = molecular weight (kg/kgmoles)

T = temperature (K)

σ = collision diameter (angstroms)

Ω_μ = collision integral (dimensionless)

The collision integral is a function of the dimensionless temperature, $\frac{k_B T}{\varepsilon}$, as shown in Figure 1 [3]:

$$\Omega_\mu = f\left(\frac{k_B T}{\varepsilon}\right) \quad (2)$$

where: k_B = Boltzmann constant (1.38049×10^{-23} J/K)

T = temperature (K)

ε = characteristic energy of interaction between molecules (J)

Excellent curve-fits to the data in Figure 1 are given by the following formulae [4]:

$$\ln \Omega_\mu = 0.557 - 0.145 \ln\left(\frac{k_B T}{\varepsilon}\right) - 0.405 |\operatorname{erf}(S_\mu)| \quad \text{if} \quad \frac{k_B T}{\varepsilon} \leq 6 \quad (3)$$

$$\Omega_\mu = 1.1615 \left(\frac{k_B T}{\varepsilon}\right)^{-0.1487} \quad \text{if} \quad \frac{k_B T}{\varepsilon} > 6 \quad (4)$$

Expressions for estimating the thermal conductivity of a gas must take into account whether the gas is monatomic or polyatomic. For a monatomic gas, the Chapman-Enskog theory may be used to obtain an expression for the thermal conductivity [2]:

$$k = \frac{8.322 \times 10^{-2} \left(\frac{T}{M}\right)^{0.5}}{\sigma^2 \Omega_\mu} \quad (\text{monatomic gas}) \quad (5)$$

where: k = thermal conductivity (W/m-K)

M = molecular weight (kg/kgmoles)

T = temperature (K)

σ = collision diameter (angstroms)

Ω_μ = collision integral (dimensionless)

For a polyatomic gas, the thermal conductivity may be estimated by using the modified Eucken correlation [2]:

$$k = \frac{\mu R}{M} \left[1.32 \left(\frac{C_p M}{R} - 1 \right) + 1.77 \right] \quad (\text{polyatomic gas}) \quad (6)$$

where: k = thermal conductivity (W/m-K)

μ = Newtonian viscosity (kg/m-s)

R = universal gas constant (8314 J/kgmole-K)

M = molecular weight (kg/kgmoles)

C_p = constant pressure heat capacity (J/kg-K)

While the heat capacity tends to be nearly constant for monatomic gases, it may vary with temperature for polyatomic gases and can be expressed in terms of a polynomial in temperature. Such an expression, however, would result in expressions too complex for the purposes of this paper. When ideal gas behavior is assumed, simple expressions may be used for the heat capacity of monatomic and diatomic gases [5]:

$$C_p = \frac{5R}{2M} \quad (\text{monatomic gas}) \quad (7)$$

$$C_p = \frac{7R}{2M} \quad (\text{diatomic gas}) \quad (8)$$

where: C_p = constant pressure heat capacity (J/kg-K)

R = universal gas constant (8314 J/kgmole-K)

M = molecular weight (kg/kgmoles)

Using equations (1), (5), (6), (7), and (8), the viscosity, thermal conductivity, and heat capacity for argon, helium, hydrogen, and nitrogen were estimated at the temperatures 280 K, 500 K, 1000 K, 1500 K, and 2000 K. The estimated values were compared with published values [5-7] in Figures 2-5. The estimated values for argon appear to be quite good, being within 5%, 7%, and 0.1% for viscosity, thermal conductivity, and heat capacity, respectively. For helium, the estimated viscosity is within 6% of the published value. The estimated thermal conductivity is within 3% of the published value at 280 K. Data points for the thermal conductivity at 1500 K, 2000 K, and 2500 K had to be extrapolated. The difference between the curves is about 22% at 2500 K; this difference arises both from the estimation technique and the extrapolation, but the extent of the contribution of each one is unknown. The published values for the heat capacity are those given by equation (7), so the estimated and published values are the same.

For hydrogen, the difference between the viscosity curves is less than 11%, less than 24% for the thermal conductivity curves, and less than 12% for the heat capacity curves. Extrapolated values were used for viscosity and heat capacity at 2500 K, and for thermal conductivity at 2000 K and 2500 K. For nitrogen, the viscosity curves differ by less than 6%, the thermal conductivity curves by less than 24%, and the heat capacity curves by less than 19%. Extrapolated values were used for viscosity and heat capacity at 2500 K. The differences between the curves for both hydrogen and nitrogen result from both the estimation and the extrapolation. Again, the individual contributions of each is unknown.

Equation (6) for the thermal conductivity, known as the modified Eucken correlation, usually predicts values which are higher than those observed experimentally [2]. While the estimated values for the four gases examined here are higher than published values at lower temperatures, they are lower than the published values at the higher temperatures.

Since the purpose of this paper is to be able to get a rough idea of the type of flow inside a CVD reactor at various conditions, the errors in the estimated values for the thermophysical properties are low enough to allow a useful analysis.

3. EXPRESSIONS FOR DIMENSIONLESS NUMBERS

The Prandtl number is the ratio of the Newtonian fluid properties [8]:

$$Pr \equiv \frac{\nu}{\alpha} = \frac{\mu C_p}{k} \quad (9)$$

Substituting (1), (5), and (7) into (9) yields a constant for the Prandtl number:

$$Pr = 0.667 \quad (\text{monatomic gas}) \quad (10)$$

Substituting (1), (6), and (8) into (9) yields a constant for the Prandtl number:

$$Pr = 0.690 \quad (\text{diatomic gas}) \quad (11)$$

The Knudsen number is used to determine if a continuum approach is valid in analyzing a system. Generally, continuum fluid dynamics can be used to study flow for $Kn < 0.01$. For $0.01 < Kn < 10$, the flow is transitional. For $Kn > 10$, a molecular approach must be used to describe the flow [9]. The Knudsen number is expressed as:

$$Kn = \frac{\lambda}{L} \quad (12)$$

where: λ = mean free path (m)

L = characteristic length (m)

In a dilute gas mixture in which species B is the predominant gas, any of the other species will most likely collide with a molecule of species B. The distance a molecule of A travels before colliding with molecule B may be expressed as [10]:

$$\lambda = \frac{4V}{\pi N_B (\sigma_A + \sigma_B)^2} \left(\frac{M_A + M_B}{M_B} \right)^{-0.5} \quad (13)$$

where: V = volume (m^3)

M_A = molecular weight of species A

M_B = molecular weight of species B

N_B = number of molecules of species B

σ_i = collision diameter (angstroms)

Using the equation of state for an ideal gas, the quantity $\frac{N_B}{V}$ may be expressed as:

$$\frac{N_B}{V} = \frac{x_B P A_0}{RT} \quad (14)$$

where: N_B = number of molecules of species B

V = volume (m^3)

x_B = mole fraction of species B

P = pressure (Pascals)

A_0 = Avogadro's number (6.023×10^{26} /kgmole)

R = universal gas constant (8314 J/kgmole-K)

T = temperature (K)

Substituting equations (13), and (14) into equation (12) yields:

$$Kn = \frac{4R}{\pi A_0} \left(\frac{M_A + M_B}{M_B} \right)^{-0.5} \frac{1}{(\sigma_A + \sigma_B)^2} \left(\frac{1}{L} \right) \left(\frac{T}{x_B P} \right) \quad (15)$$

By multiplying out the constants, with appropriate corrections for using the more common units of Angstroms for σ_i instead of meters, the final expression for the Knudsen number is obtained:

$$Kn = 1.758 \times 10^{-3} \left[\left(\frac{M_A + M_B}{M_B} \right)^{-0.5} \frac{1}{(\sigma_A + \sigma_B)^2} \right] \left(\frac{1}{L} \right) \left(\frac{T}{x_B P} \right) \quad (16)$$

The Reynolds number is the controlling parameter for forced convection. In pipe flow, for instance, the flow is always laminar for a Reynolds number less than 2000 [11]. Forced convection can be neglected if $(Re \cdot Pr)^{0.5} \ll 1$ [11]. The Reynolds number is given by:

$$Re = \frac{\langle v \rangle L}{\nu} \quad (17)$$

where: $\langle v \rangle$ = average velocity (m/s)

L = characteristic length (m)

ν = kinematic viscosity (m^2/s)

The kinematic viscosity may be expressed as [1]:

$$\nu = \frac{\mu}{\rho} \quad (18)$$

where: μ = Newtonian viscosity (kg/m-s)

ρ = density (kg/m^3)

From the equation of state for an ideal gas, density may be expressed as:

$$\rho = \frac{PM}{RT} \quad (19)$$

where: ρ = density (kg/m^3)

P = pressure (Pa)

M = molecular weight (kg/kgmole)

R = universal gas constant (8314 J/kgmoles-K)

T = temperature (K)

The average velocity may be obtained by summing all velocities over a cross-section, then dividing by the cross-sectional area [1]. Such an expression would be too complex for the purposes of this paper. For a reactor with a constant cross-sectional area, the mass flow rate into the reactor for steady flow may be expressed as:

$$\dot{m} = \rho \langle v \rangle A_{CS} \quad (20)$$

where: \dot{m} = mass flow rate (kg/s)

ρ = density (kg/m^3)

$\langle v \rangle$ = average velocity (m/s)

A_{cs} = cross-sectional area (m^2)

By substituting equation (19) into equation (20) and rearranging the terms, and approximation for the average velocity is obtained:

$$\langle v \rangle = \frac{\dot{m}RT}{PMA_{CS}} \quad (21)$$

where: $\langle v \rangle$ = average velocity (m/s)
 \dot{m} = mass flow rate (kg/s)
 R = universal gas constant (8314 J/ kgmoles-K)
 T = temperature (K)
 P = pressure (Pa)
 M = molecular weight (kg/kgmole)
 A_{cs} = cross-sectional area (m²)

In order to obtain the average velocity, the mass flow rate, \dot{m} , should be the average mass flow rate through the reactor. Since many CVD reactors use a dilute solution of reactive species in a carrier gas, the mass flow into the reactor is essentially equal to the mass flow out of the reactor. In this case, the average mass flow rate should be essentially equal to the inlet mass flow rate, which can be obtained from the settings of the mass flow controllers for the reactor.

Substituting equations (1), (18), (19), and (21) into equation (17) yields:

$$Re = 3.747 \times 10^5 \left(\frac{\sigma^2 \Omega_\mu}{M^{0.5}} \right) \left(\frac{L}{A_{CS}} \right) \left(\frac{\dot{m}}{T^{0.5}} \right) \quad (22)$$

The Peclet number is the thermal equivalent of the Reynolds number. Forced convective heat transfer can be neglected if $Pe^{0.5} \ll 1$ [8]. The Peclet number may be expressed as:

$$Pe = \frac{\langle v \rangle L}{\alpha} \quad (23)$$

where: $\langle v \rangle$ = average velocity (m/s)

L = characteristic length (m)

α = thermal diffusivity (m^2/s)

The thermal diffusivity is defined as:

$$\alpha = \frac{k}{\rho C_p} \quad (24)$$

where: k = thermal conductivity (W/ m-K)

ρ = density (kg/m^3)

C_p = constant pressure heat capacity (J/kg-K)

An expression for the Peclet number for a monatomic gas may be obtained by substituting equations (5), (7), and (19) into (24), then this result, along with (21), into (23):

$$Pe = 2.498 \times 10^5 \left(\frac{\sigma^2 \Omega_\mu}{M^{0.5}} \right) \left(\frac{L}{A_{CS}} \right) \left(\frac{\dot{m}}{T^{0.5}} \right) \quad (\text{monatomic gas}) \quad (25)$$

Similarly, an expression for the Peclet number for a diatomic gas may be obtained by substituting equations (6), (8), and (19) into (24), then this result, along with (21), into (23):

$$Pe = 2.586 \times 10^5 \left(\frac{\sigma^2 \Omega_\mu}{M^{0.5}} \right) \left(\frac{L}{A_{CS}} \right) \left(\frac{\dot{m}}{T^{0.5}} \right) \quad (\text{diatomic gas}) \quad (26)$$

The Grashof number, which may be interpreted as the ratio of the momentum flux by free convection to that by diffusion, is useful in determining the magnitude of free convective effects. The Grashof number plays the same role in free convection as the Reynolds number does in forced convection [12]. No turbulence is expected for a Grashof number well below 1×10^5 [13]. The ratio Gr/Re^k is often used to describe the occurrence of buoyancy effects.

The value of κ can depend on the reactor configuration and the value of the Reynolds number.

The Grashof number may be expressed as [1]:

$$Gr = \frac{g\beta_T L^3 \Delta T}{\nu^2} \quad (27)$$

where: g = gravitational constant (9.8 m/s^2)

β_T = coefficient of volume expansion (K^{-1})

L = characteristic length (m)

ΔT = characteristic temperature difference (K)

ν = kinematic viscosity (m^2/s)

β_T is defined as:

$$\beta_T = -\frac{1}{\rho} \left(\frac{\partial \rho}{\partial T} \right)_P \quad (28)$$

Assuming an ideal gas, β_T becomes equal to $1/T$.

By substituting equations (1), (18), (19), and (28) into equation (27), the following equation is obtained:

$$Gr = 2.031 \times 10^3 g (M\sigma^4 \Omega_\mu^2) (L^3) \left(\frac{\Delta T P^2}{T^4} \right) \quad (29)$$

When $g = 9.8 \text{ m/s}$, equation (29) becomes:

$$Gr = 1.9903 \times 10^4 (M\sigma^4 \Omega_\mu^2) (L^3) \left(\frac{\Delta T P^2}{T^4} \right) \quad (30)$$

The Rayleigh number, which may be interpreted as the ratio of the thermal flux by free convection to that by diffusion, characterizes the convective state of an enclosed gas subjected to a destabilizing temperature gradient, such as a heated bottom and cold upper wall [14]. This is often the situation in horizontal CVD reactors with walls actively-cooled by water and a heated deposition surface. Natural convective heat transfer can be neglected if $(Ra \cdot Pr)^{0.25} \ll 1$ [8]. Longitudinal convective rolls have been found to appear in horizontal CVD reactors for $Ra > 1708$. The transition from laminar to turbulent flow occurs at Ra greater than about 2300 [15]. The Rayleigh number may be expressed as:

$$Ra = \frac{g\beta_T L^3 \Delta T}{\nu \alpha} \quad (31)$$

where: g = gravitational constant (m/s^2)

β_T = coefficient of volume expansion (K^{-1})

L = characteristic length (m)

ΔT = characteristic temperature difference (K)

ν = kinematic viscosity (m^2/s)

α = thermal diffusivity (m^2/s)

By substituting equations (1), (5), (7), (18), (19), (24), and (28) into equation (31), an expression of the Rayleigh number for a monatomic gas is obtained:

$$Ra = 1.354 \times 10^3 g (M\sigma^4 \Omega_\mu^2) (L^3) \left(\frac{\Delta T P^2}{T^4} \right) \quad (\text{monatomic gas}) \quad (32)$$

When $g = 9.8 \text{ m/s}$, equation (32) becomes:

$$Ra = 1.3267 \times 10^4 (M\sigma^4 \Omega_\mu^2) (L^3) \left(\frac{\Delta T P^2}{T^4} \right) \quad (\text{monatomic gas}) \quad (33)$$

By substituting equations (1), (6), (8), (18), (19), (24), and (28) into equation (31), an expression for the Rayleigh number for a diatomic gas is obtained:

$$Ra = 1.402 \times 10^3 g (M \sigma^4 \Omega_\mu^2) (L^3) \left(\frac{\Delta T P^2}{T^4} \right) \quad (\text{diatomic gas}) \quad (34)$$

When $g = 9.8 \text{ m/s}$, equation (34) becomes:

$$Ra = 1.3739 \times 10^4 (M \sigma^4 \Omega_\mu^2) (L^3) \left(\frac{\Delta T P^2}{T^4} \right) \quad (\text{diatomic gas}) \quad (35)$$

A comparison of equations (17) and (23) shows that the Reynolds number and Peclet number differ only in their denominators; comparing equations (27) and (31) shows that the Grashof and Rayleigh numbers also differ only in their denominators. Since the momentum diffusivity, ν , and the energy diffusivity, α , are always of the same order of magnitude for gases [11], it is expected that substitution of expressions for these quantities into expressions for the dimensionless numbers would yield essentially identical expressions for the Reynolds number and Peclet number (as a comparison of equation (22) with equations (25) and (26) shows), as well as essentially identical expressions for the Grashof and Rayleigh numbers (as a comparison of equation (29) with equations (32) and (34) shows).

All the dimensionless numbers examined in this paper have temperature as a variable in their expressions. The temperature varies widely in a CVD reactor, making it difficult to determine the temperature to use in calculating the numbers. Since the material is deposited on a substrate surface, flow patterns over this deposition surface will often be of the most interest. As an approximation, the temperature used to calculate the dimensionless numbers may be taken as the average between the reactor wall and the substrate surface:

$$T = \frac{T_{\text{sub}} + T_{\text{wall}}}{2} \quad (36)$$

where: T_{sub} = substrate surface temperature (K)

T_{wall} = reactor wall temperature (K)

The expressions for the Grashof and Rayleigh numbers contain a temperature difference. Again, since the main area of interest is likely to be over the deposition surface, the temperature difference can be taken to be the difference in temperature between the reactor wall and deposition surface:

$$\Delta T = T_{\text{sub}} - T_{\text{wall}} \quad (37)$$

where: T_{sub} = substrate surface temperature (K)

T_{wall} = reactor wall temperature (K)

5. SAMPLE CALCULATIONS USING ESTIMATION EXPRESSIONS

As an example of the use of the various estimation expressions, consider a very simple horizontal CVD reactor with a square cross-section, 0.05 meters on a side. The top and side walls are maintained at a temperature of 280 K, while the bottom wall, where the substrate surface is located, is maintained at a temperature of 1800 K. The gas in the reactor consists of an helium carrier gas with a mole fraction of silane equal to 3×10^{-4} . The operating pressure is 1.01325×10^5 Pa. The mass flow rate into the reactor is equal to 2.3×10^{-5} kg/s.

To begin, values for various parameters needed to calculate the dimensionless numbers will be obtained from the given conditions:

$$x_B = 1 - 3 \times 10^{-4} = 9.997 \times 10^{-1}$$

$$A_{CS} = 0.05 \times 0.05 = 2.5 \times 10^{-3} \text{ m}^2$$

$$\text{From (36): } T = (280 + 1800)/2 = 1040 \text{ K}$$

$$\text{From (37): } \Delta T = 1800 - 280 = 1520 \text{ K}$$

$$\text{From (21): } \langle v \rangle = (2.3 \times 10^{-6})(8314)(1040)/(1.01 \times 10^{-5})(4.003)(2.5 \times 10^{-3}) = 2 \times 10^{-2} \text{ m/s}$$

$$\frac{k_B T}{\epsilon} = 1040 / 10.2 = 102; \text{ therefore, use (4) to calculate } \Omega_\mu :$$

$$\Omega_\mu = 1.1615(102)^{-0.1487} = 0.584$$

Except for the Knudsen number, which uses physical parameter values for both helium and silane, the physical parameters of helium are used in all calculations. Since the silane is present in such a low concentration, the properties of the gas in the reactor are essentially those of helium.

In calculating the Knudsen number, let species A be silane and species B be helium. Physical parameters for helium may be found in Table 3. For silane [16]:

$$M = 32.1 \text{ kg/kgmole}$$

$$\sigma = 4.084 \text{ angstroms}$$

$$\epsilon/k_B = 207.6 \text{ K}$$

Equation (16) is used to calculate the Knudsen number: $Kn = 3 \times 10^{-6}$. This value implies that continuum fluid dynamics can be used to study the flow.

The Reynolds number is calculated from equation (22): $Re = 1$. This value implies that the flow in the reactor will be laminar. $(Re \cdot Pr)^{0.5} = 0.8$, which indicates that forced convection cannot be neglected in this problem.

The Peclet number is calculated from equation (25): $Pe = 7$. This value indicates that heat transfer by convection and diffusion are about the same order of magnitude. This is

confirmed by $Pe_{eff} = 0.8$, which shows that forced convection heat transfer cannot be ignored.

The Grashof number is calculated from equation (30): $Gr = 2000$. Turbulent flow is not expected for this value of the Grashof number.

The Rayleigh number is calculated from equation (33): $Ra = 1300$. No longitudinal convective rolls should occur; however, this value is getting close enough to the critical value of $Ra = 1708$ that it is not inconceivable that such rolls would be present. The equations used to calculate these numbers contain a number of simplifying assumptions, and cannot be expected to yield exact results. $(Ra \cdot Pr)^{0.25} = 6$, which implies that free convective heat transfer cannot be ignored.

4. EVALUATION OF EXPRESSIONS FOR DIMENSIONLESS NUMBERS

Values for dimensionless numbers calculated using the expressions in this paper were verified against previously published values that were calculated using thermophysical properties obtained from a computational model of a CVD reactor [17]. The comparison is shown in Table 2. Molecular weights and values for the collision diameter used to compute the dimensionless numbers are shown in Table 3. The values computed using the expressions in this paper agreed well with those computed from values obtained from the computational model, such as thermophysical properties, average temperature, and average velocity. Since both the computational model and the expressions above calculated these parameters using estimation expressions based on kinetic theory, their agreement serves as a check on the derivation of the expressions for dimensionless numbers in terms of process parameters.

5. CONCLUSIONS

Dimensionless numbers useful for analyzing flow in CVD systems have been expressed in terms of parameters commonly under the control of the system operator, such as temperature and pressure. These expressions clearly indicate the dependence of these numbers on system parameters, and allow a quick determination of the flow regime inside the reactor that is sufficiently accurate for many applications. These expressions also allow a quick determination of the sensitivity of the flow to changes in system parameters.

NOTATION

<u>Symbol</u>	<u>Description</u>	<u>Units</u>
A_{cs}	cross-sectional area	m^2
A_0	Avogadro's number	$kgmole^{-1}$
C_p	constant pressure heat capacity	$J/kg-K$
g	gravitational constant	m/s^2
k	thermal conductivity	$W/m-K$
k_B	Boltzmann constant	J/K
L	characteristic length	m
M_i	molecular weight	$kg/kgmoles$
N_i	number of molecules of species i	molecules
P	pressure	Pa
R	universal gas constant	$J/kgmoles-K$
T	temperature	K
ΔT	characteristic temperature difference	K
V	volume	m^3
x_i	mole fraction of species i	dimensionless
α	thermal diffusivity	m^2/s
β_T	coefficient of volume expansion	K^{-1}
ϵ	characteristic energy of interaction between molecules	J
κ	exponent in ratio Gr/Re^κ	dimensionless
μ	Newtonian viscosity	$kg/m-s$
ρ	density	kg/m^3
σ	collision diameter	angstroms
ν	kinematic viscosity	m^2/s
Ω_μ	collision integral for viscosity and thermal conductivity	dimensionless

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Table 1: Dimensionless numbers useful in CVD flow analysis

Name	Description	Physical Interpretation
Prandtl	$Pr = \frac{\mu}{\alpha}$	$\frac{\text{momentum diffusivity}}{\text{thermal diffusivity}}$
Knudsen	$Kn = \frac{\lambda}{L}$	$\frac{\text{mean free path}}{\text{characteristic length}}$
Reynolds	$Re = \frac{\langle v \rangle L}{\nu}$	$\frac{\text{momentum flux by convection}}{\text{momentum flux by diffusion}}$
Peclet (thermal)	$Pe = \frac{\langle v \rangle L}{\alpha}$	$\frac{\text{thermal flux by convection}}{\text{thermal flux by diffusion}}$
Grashof (thermal)	$Gr = \frac{g\beta_T L^3 \Delta T}{\nu^2}$	$\frac{\text{momentum flux by free convection}}{\text{momentum flux by diffusion}}$
Rayleigh (thermal)	$Ra = \frac{g\beta_T L^3 \Delta T}{\nu \alpha}$	$\frac{\text{thermal flux by free convection}}{\text{thermal flux by diffusion}}$

Table 2: Comparison of dimensionless numbers

Dimensionless Number	Equation Used	Estimated (P=2.7 kPa)	Estimated (P=101 kPa)	Model [17] (P=2.7 kPa)	Model [17] (P=101 kPa)
Pr	(11)	6.9×10^{-1}	6.9×10^{-1}	1	1
Kn	(16)	2×10^{-4}	6×10^{-6}	1×10^{-4}	1×10^{-6}
Re	(21)	2	2	3	3
Pe	(25)	2	2	1	1
Gr	(28)	0.2	200	0.2	200
Ra	(33)	0.1	150	0.2	200

Table 3: Physical parameters for gases [1]

Gas	M (kg/kgmoles)	σ (Angstroms)	ε/k_B (K)
argon	39.944	3.418	124.0
helium	4.003	2.576	10.2
hydrogen	2.016	2.915	38.0
nitrogen	28.02	3.681	91.5

Figure 1: Collision integral for viscosity and thermal conductivity calculations as a function of dimensionless temperature for the range: a) $0 < \frac{k_B T}{\epsilon} < 10$; b) $10 < \frac{k_B T}{\epsilon} < 400$.

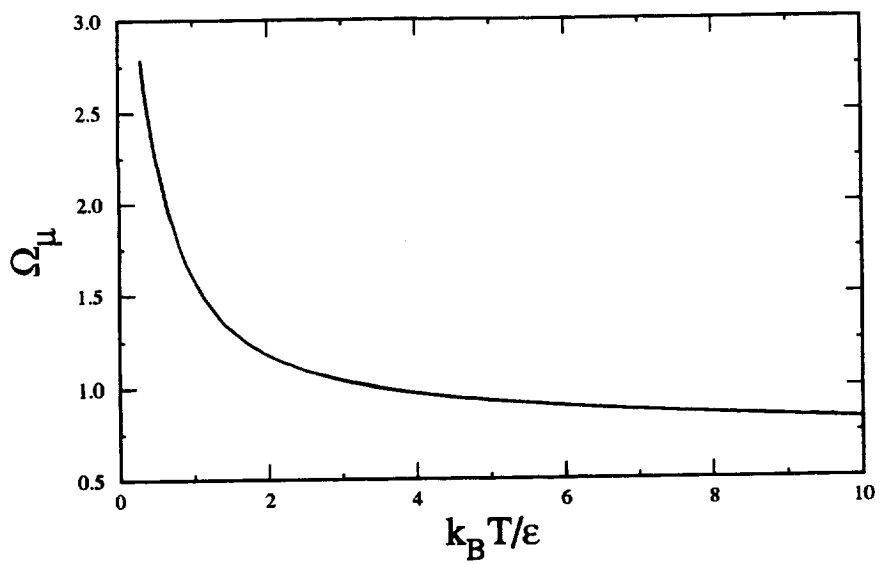
Figure 2: Comparison of estimated and published property values for argon [5-7]: a) viscosity; b) thermal conductivity; c) heat capacity.

Figure 3: Comparison of estimated and published property values for helium [5-7]: a) viscosity; b) thermal conductivity; c) heat capacity. The estimated and published values for helium heat capacity are the same.

Figure 4: Comparison of estimated and published property values for hydrogen [5-7]: a) viscosity; b) thermal conductivity; c) heat capacity.

Figure 5: Comparison of estimated and published property values for nitrogen: a) viscosity; b) thermal conductivity; c) heat capacity.

a)



b)

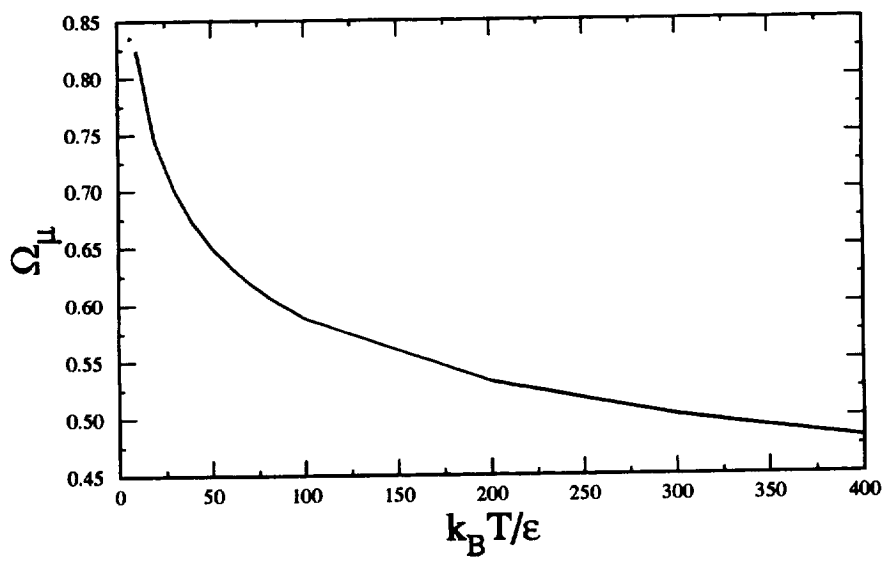


Figure 1

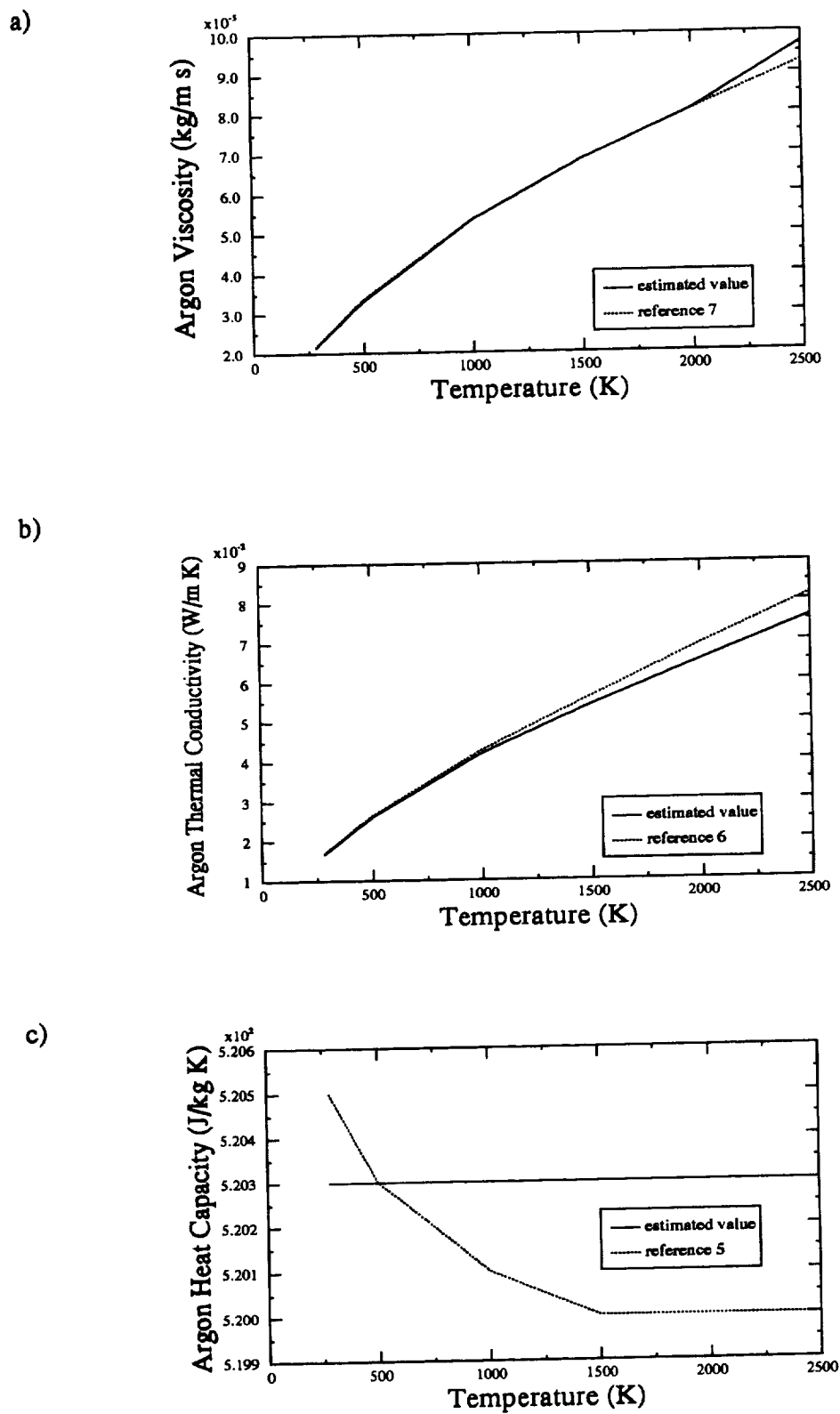
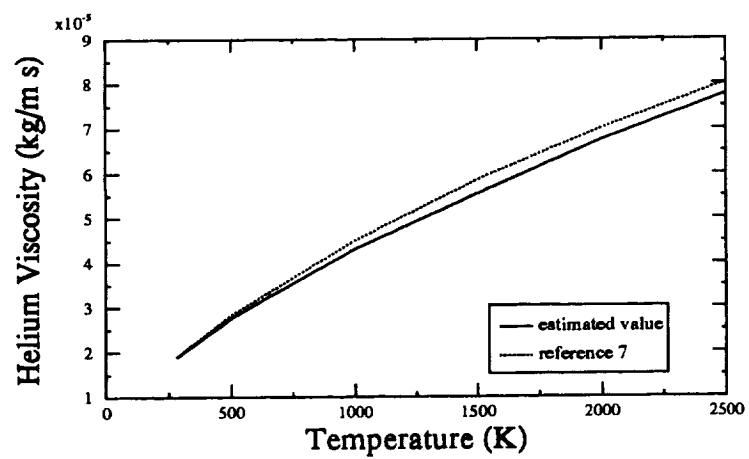
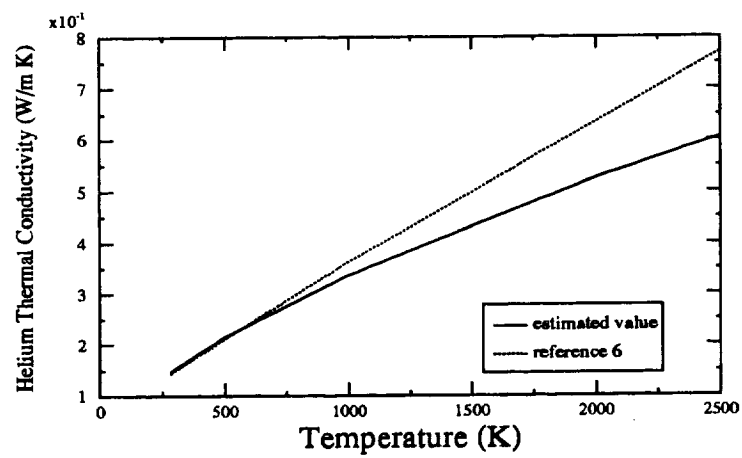


Figure 2

a)



b)



c)

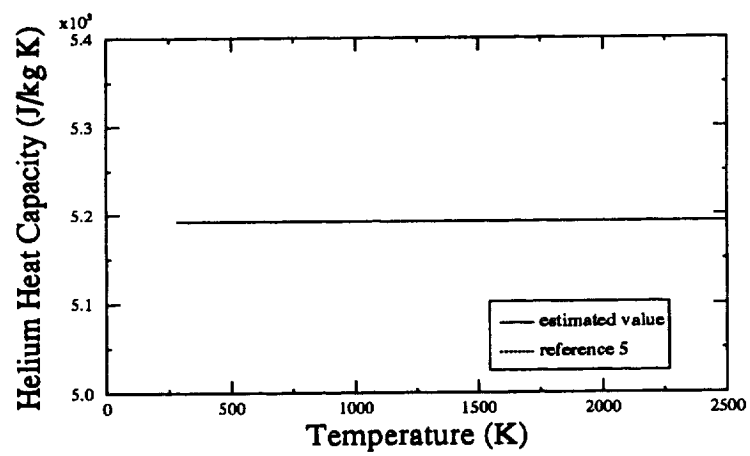
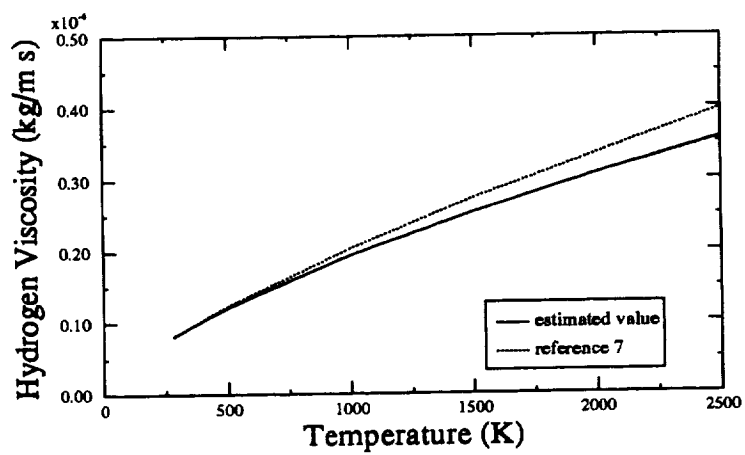
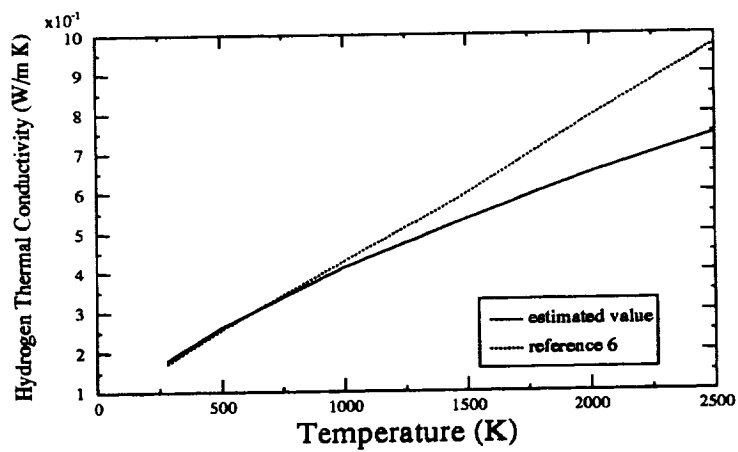


Figure 3

a)



b)



c)

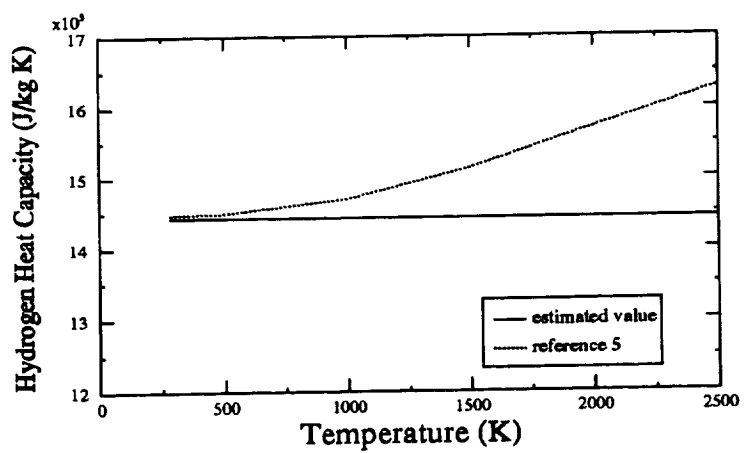
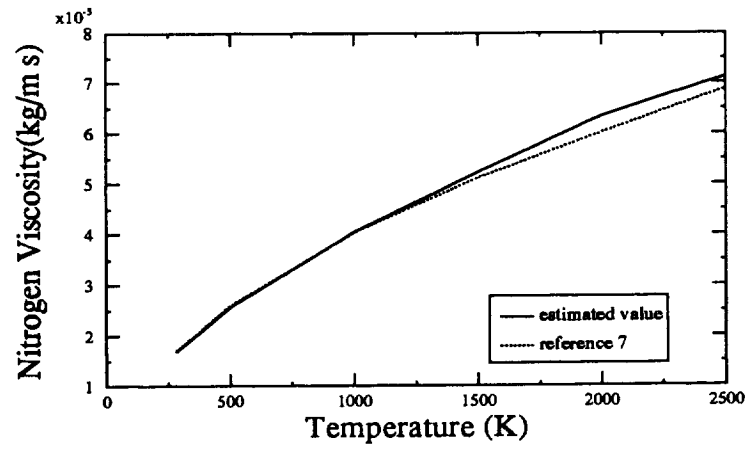
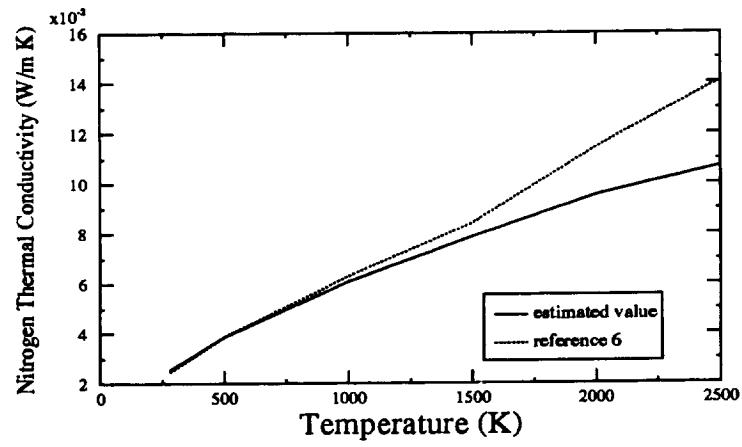


Figure 4

a)



b)



c)

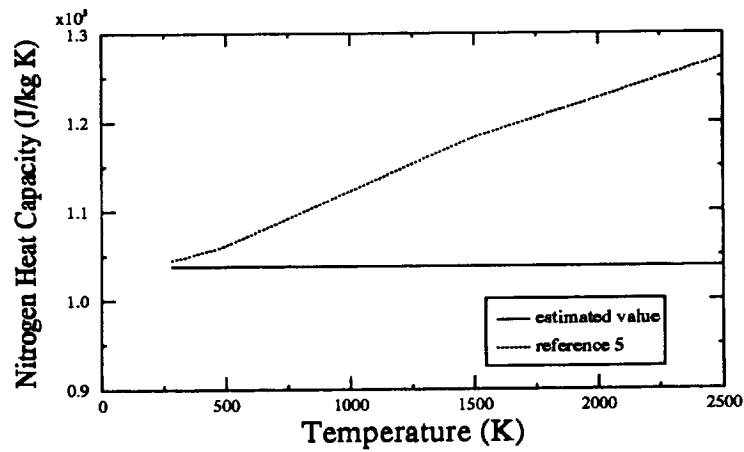


Figure 5

