Fundamentals of Combustion

Prof. V. Raghavan
Department of Mechanical Engineering
Indian Institute of Technology, Madras

Lecture - 26

Governing Equations for Reacting Flow – Part 3

Estimation of Thermo-Physical Properties and Control of Combustion Phenomena

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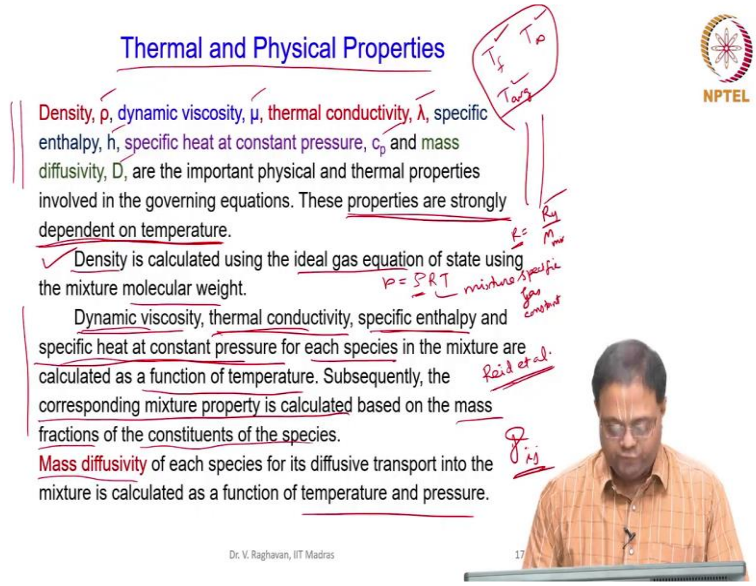

Thermal and Physical Properties

Density, ρ, dynamic viscosity, μ, thermal conductivity, λ, specific enthalpy, h, specific heat at constant pressure, c_p and mass diffusivity, D, are the important physical and thermal properties involved in the governing equations. These properties are strongly dependent on temperature.

Density is calculated using the ideal gas equation of state using the mixture molecular weight.

Dynamic viscosity, thermal conductivity, specific enthalpy and specific heat at constant pressure for each species in the mixture are calculated as a function of temperature. Subsequently, the corresponding mixture property is calculated based on the mass fractions of the constituents of the species.

Mass diffusivity of each species for its diffusive transport into the mixture is calculated as a function of temperature and pressure.

T_f T_∞ T_{avg}

$R = \frac{R_u}{M_{mix}}$

$p = \rho R T$ mixture specific gas constant

Reid et al.

$\mathcal{D}_{ij}$

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17

Now, we will see some important properties which are required for the governing equations. The first one is density, then dynamic viscosity so momentum equation has this, then thermal conductivity energy equation has this, then the specific enthalpy of the mixture, then specific heat at constant pressure c_p, then the mass diffusivity for calculating diffusion velocities.

So, these are all the important physical and thermal parameters involved in the governing equations. Please understand that these properties depend on temperature very strongly, strong because of the significant temperature gradient which we see in the reactive flows we have to calculate the properties as a function of temperature, so that will give accurate results; but there are several approaches where we need not do that we can calculate the property at an average temperature.

See for example, if flame temperature is T_f; so flame temperature say T suffix f, and the ambient temperature is say T_∞, you can take some average temperature in between this and calculate the properties at this average temperature that is also fine. But it might not work for all the things, so for a predictive model normally you take the flame temperature, and then ambient temperature

The temperature varies in the between these two T_f to T_∞. So, as a function of temperature calculate all the properties, so properties which are strongly dependent on temperature are calculated as function of temperature. Now, the mixture properties are calculated based upon the concentration of the species in the mixture. These are the two things which actually we have to say, so this is the comprehensive approach we do this.

So, for density as I told you use the ideal gas equation of state so $p = \rho RT$, so this is the mixture specific gas constant, then this is the pressure, temperature is known this is calculated as what? So, the $R = R_u/MW_{mix}$, so you know the mixtures molecular weight.

So, universal gas constant divided by the molecular weight of the mixture will give you the specific gas constant of the mixture, so you can use that and calculate the density ρ; because ideal gas equation of state is used for that.

So, mixture molecular weight will give you the specific gas constant, so that is what I have written here. Similarly, the dynamic viscosity μ, thermal connectivity, specific enthalpy and the specific heat of constant pressure of each species.

First of all you have to calculate, so before arriving at the dynamic viscosity of the mixture we need to know the viscosities of each species. So, it should be calculated a function of temperature, so there are correlations available; you can take any standard property textbooks like Reid et al and get this.

You can get the correlations, a lot of researchers have worked on correlations for calculating the properties. So, see one of the important book is Reid et al., so this gives the properties of gases and liquids as a function of temperature and pressure; so in low pressure regime and high pressure regime, and so on. So, lot of correlations have been listed here and the research papers can be used to calculate the properties.

So, the dynamic viscosity, thermal conductivity, specific enthalpy, specific heat at constant pressure of each species in the mixture are calculated as a function of temperature first. Then mixture property can be calculated using the concentrations or mass fractions or mole fractions whatever of the constituents. So, now we are incorporating both temperature dependency plus the concentration or the mass fractions of each species.

Now, what about mass diffusivity; binary mass diffusivity D_{ij}, binary mass diffusivity of a pair of species i and j can be calculated as a function of temperature and pressure; so once you know this, you can calculate the diffusion coefficient.

So, once diffusion coefficient is known, we can calculate the diffusion velocity. Similarly, thermal diffusion coefficient also can be calculated using some correlations, and using that thermal diffusion coefficient we can calculate the diffusion velocity due to thermal diffusion, Soret effect.

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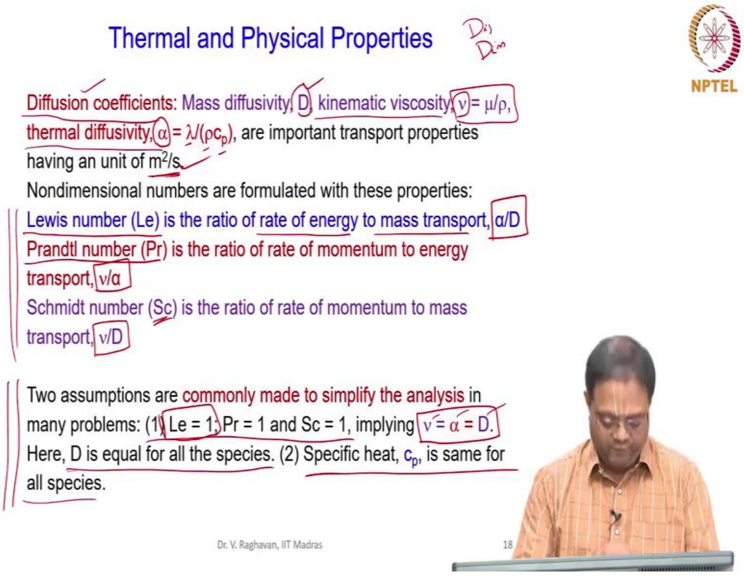

Thermal and Physical Properties

D_{ij}
D_{im}

Diffusion coefficients: Mass diffusivity, D, kinematic viscosity, $\nu = \mu/\rho$, thermal diffusivity, $\alpha = \lambda/(\rho c_p)$, are important transport properties having an unit of m^2/s.

Nondimensional numbers are formulated with these properties:

Lewis number (Le) is the ratio of rate of energy to mass transport, α/D

Prandtl number (Pr) is the ratio of rate of momentum to energy transport, ν/α

Schmidt number (Sc) is the ratio of rate of momentum to mass transport, ν/D

Two assumptions are commonly made to simplify the analysis in many problems: (1) Le = 1; Pr = 1 and Sc = 1, implying $\nu = \alpha = D$. Here, D is equal for all the species. (2) Specific heat, c_p, is same for all species.

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18

So, diffusion coefficients for the mass transfer it is the mass diffusivity; so it can be binary diffusivity or D_{im}, so some mass diffusivity say D; and not dynamic viscosity kinematic viscosity which is $\nu = \mu/\rho$, and thermal diffusivity α which is $\lambda/\rho c_p$.

So, $\lambda/\rho c_p$ that will be the thermal diffusivity which you designate the symbol α for that so ν, D and α are the diffusion coefficients and the unit for them is m^2/s. So, diffusion coefficient, this diffusion coefficient have the unit of m^2/s.

So, you can see that based upon the species, the mixture, etcetera; these properties will vary, so they may not be actually same. But what we can do is we can actually define some non-dimensional numbers based upon these three.

So, the first number what we define is called Lewis number Le, Lewis number which is the ratio of the rate of energy to the mass transport, α/D that is the Lewis number. Prandtl number, the familiar number, it is the ratio of the rate of momentum to energy transport that is ν/α.

The third number is Schmidt number, where it deals with the ratio of rate of momentum to mass transport that is ν/D, Schmidt number; so Sc. So, Le, Pr and Sc are the three non-dimensional numbers which actually deals with ratio of any two diffusion coefficient at a time and that will be a non-dimensional numbers.

Now, basically these numbers need not be the same. For example, even the α, ν and D are different; and we can say that these numbers will not be same, Lewis number can be different and Prandtl number can be different and the Schmidt number can be different, but commonly what we assume is these are all the same, so this is one of the assumptions we make.

Basically, we make this assumption Lewis number is equal to 1 that assumption we make to simplify the problem, so that we will see later; how to simplify the problem by assuming Lewis number equal to 1. So, when you assume these all the three non-dimensional numbers are unity, then what we actually assume is that diffusion coefficients for mass, momentum and the energy are the same that is D, α and ν are the same.

So, D is equal for all the species. We have also assumed that the specific heat is same for all species in several simplifying approaches, when you want to do a comprehensive analysis we actually vary all the properties as a function of temperature and arrive at the mixture property by using some mixing rules.

But when you want to simplify the problem, the non-dimensional numbers; Lewis number, Prandtl number and Schmidt number have been assumed as unity and the D, the diffusion coefficient all the species into the mixture is same and specific heat also is assumed to be same for all species So, these are the assumptions which we invoke; so why we invoke, because to simplify the problem which is otherwise complicated.

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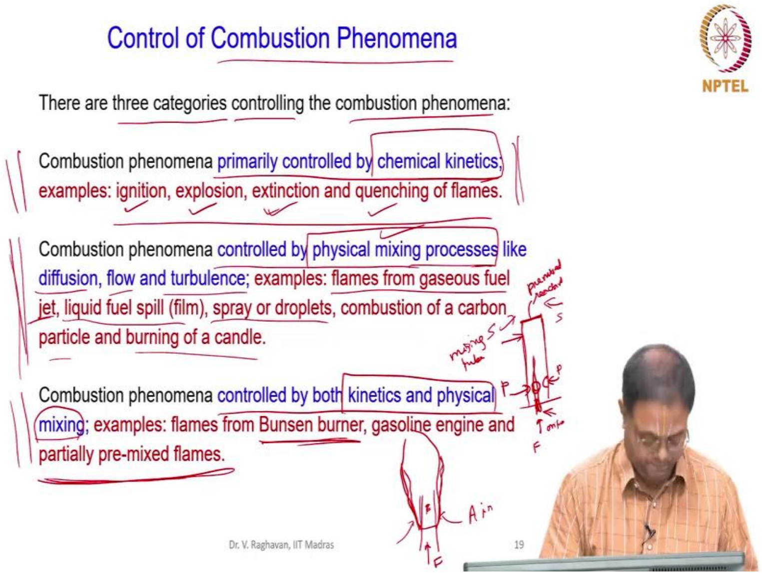

Control of Combustion Phenomena

There are three categories controlling the combustion phenomena:

Combustion phenomena primarily controlled by chemical kinetics; examples: ignition, explosion, extinction and quenching of flames.

Combustion phenomena controlled by physical mixing processes like diffusion, flow and turbulence; examples: flames from gaseous fuel jet, liquid fuel spill (film), spray or droplets, combustion of a carbon particle and burning of a candle.

Combustion phenomena controlled by both kinetics and physical mixing; examples: flames from Bunsen burner, gasoline engine and partially pre-mixed flames.

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19

Now, let us see when there is a combustion phenomena what are the controlling aspects in that. There are three categories controlling the combustion process, what are they; first one is a combustion phenomena can be primarily controlled by using chemical kinetics only. The rate at which the reaction takes place that will control the combustion phenomena, so this is the first category.

Example for this category is when you do a ignition, when you have a pre mixed fuel and air and you try to ignite it. So, almost a uniform mixture is prevailing here it is at a uniform temperature. So, everything is uniform here only when you ignite it, what happens is the rate at which the reaction occurs that will be the rate at which the mixture is depleted, so ignition.

Similarly, there is a premixed charge in a constant volume vessel. Now, if you ignite it pressure builds up and it explodes, so the explosion. Similarly, when the flame is propagating, it may extinguish, so the extinction flame extinction or when the flame propagates through the very small diameter tubes, it may be quenched.

It may lose heat more than what it generates; so it may be quenched. So, these are the phenomena, so this extinction basically depends upon the convective flow plus stress, the stretch of the flame, etcetera.

The quenching is due to the heat loss from the flame towards the ambient and so on. So, when you want to capture or analyze these phenomena like ignition, explosion, extinction, quenching, etcetera. Then you have to understand that these phenomena are predominantly controlled by chemical kinetics, category one. So, we do not need to understand anything else, we need to focus only on the chemical kinetics to understand these phenomena.

Second one is the combustion phenomena controlled by physical mixing processes, how the reactants species like fuel, oxidizer are mixed, how they are supplied first of all. So, whether the supply is very slow in nature for example, very slow velocity with which the reactants are coming in, so the diffusion process is going to control that.

Similarly, if there is a very high speed flow or if the flow is laminar or turbulent, these are all physical mixing process, diffusion between two species allowing them to mix; similarly, a flow of a reactant, say fuel and oxidizer coming and they are mixed due to the flow of them. Similarly, turbulent vortices of different scales which is present in the turbulent flow that will increase the rate at which the reactants are mixed.

So, the physical mixing processes would control this second category of combustion phenomena, here examples are flames from gaseous fuel jet. So, for example, I will tell you this, I will draw a burner, so this is the burner or a nozzle through which fuel is fed, so F is a fuel. So, fuel is fed through this and fuel comes out, when it comes out basically it takes in air; so this is the fuel stream F and the air airstream from the ambient, air from ambient in entrains into this fuel jet and mixes.

So, somewhere in this layer what I am drawing here, what you get is well mixed, stoichiometrically mixed reactant. So, some fuel and required oxygen is available at this portion; when you ignite this, you will get a flame so the flame will be formed. So, this is the gaseous jet, a fuel jet is coming out, there is no mixing there is no pre mixing here.

Only fuel is coming out of a port or a nozzle and due to the momentum of this jet, fuel jet which is coming out the air from the ambient entrains into this. So, physically you can see that this entrainment is due to the momentum of the jet which is coming out of this into the ambient, which is not having any flow. So, predominantly by diffusion what happens is there is a mixing of fuel and oxidizer, so physical mixing process due to diffusion.

Now, similarly if you have a liquid fuel spilled on a surface or anything, you can ignite it; so it will have a diffusion flame over this. That means, the fuel will vaporize and that will contribute to the flame which is formed.

Similarly, air from the ambient will come the other direction and mix; you can see that the rate at which the fuel vapor and the air from the ambient mixes that will control the combustion phenomena, so that this, you can see one example.

The droplet, spray of droplets; if you inject a liquid at high pressure, it will disintegrate into small droplets and each droplet will have some flame over it. For example, the droplets are bigger enough, so that some vapors are formed over surface and they mix with the ambient air, and the flame can form over the liquid droplet itself. So, this again the rate at which the vapor is going to mix with the ambient air that will control the process

Similarly, the combustion of carbon particle or burning of a candle. Best example you have seen is the burning of candle, that is a flame where you do not have any dependency on chemical kinetics, little bit dependency only. The predominant control is due to the physical mixing processes.

First the wax should melt, the molten wax should vaporize and that vapor should mix with the ambient air and that will form a flame, so this is what is the second category where the chemical kinetics is not going to control, because that is very fast. So, which is slow will control, what is slow process here, the physical mixing of the reactants that is a slower process that is going to control the entire combustion phenomena.

Now, third category obviously is the combination of these two; in some cases we cannot neglect kinetics or we cannot neglect the physical mixing process. In the first case, when only chemical kinetics is going to control; I do not really need to worry about the mixing, because already the reactants are mixed, mixing has already taken place.

Similarly, maybe the mixing is very fast so that the mixing time is very fast so that is not going to control, the chemical kinetics, the rate at which the reactant burn is going to control, so that is first category.

Second category, here the mixing process is slower now. So, the kinetics is very fast; the flame has formed, but the flame has to really form based upon the location where the fuel and the oxidizer are going to mix at the stoichiometric proportions, so that is the second category.

Third category controlled by both kinetics and physical mixing. So, now for this the example is given as Bunsen burner or a gasoline engine, spark ignition engine in automobiles are partially pre-mixed flames.

See for example, in Bunsen burner what happens is, this is the Bunsen burner, so this is the fuel supply orifice. Orifice is a nozzle, through the nozzle fuel is supplied, so there are holes in the periphery of this is a mixing tube; so this is the mixing tube and there are holes in the mixing tube, when the fuel is injected like this due to the high momentum of the fuel jet, the air entrains from the ambient.

So, there are holes in the mixing tube through the holes the air entrains and these two mix; the fuel jet entrains the air and mixes with the air. So, now what you see in the top of this tube mixing tube is a pre-mixed reactant; but this reactant is not completely premixed as we see in the first case, it may be premixed to some extent.

So, probably to the rich side it may have more fuel than stoichiometric fuel value. So, this is the Bunsen burner case where you allow the air to entrain and partially premix, so we get partially premixed flames. So, in this both the mixing rate of the additional air which is going to come out here there is additional air which is going to come in at the top of the tube mixing tube.

This is the primary air, this I will say P and S; this is P and S, P indicates primary air entraining into the mixing tube due to the momentum of the fuel jet, secondary air will entrain at the top of the burner.

So, both mixing and kinetics are important because of partially premixing kinetics is important, because of the additional air requirement the secondary air is supplied, its entrained again and physical mixing will play a role. So, both kinetics and the physical mixing plays a role in the third category, so these are the three things we should understand.

So, three categories of combustion are the combustion phenomena which is completely controlled only by chemical kinetics. Second one is it is controlled only by the physical mixing process that is the rate at which the fuel and oxidizer are transported into the combustion chamber, so that this transfer process may not be only convection; it may be diffusion or it may be turbulent everything.

Then the third one, both are important that is there are some aspects which will need kinetics to involve; there are some aspect which will need mixing process to be taken care. So, both are important in the third category.

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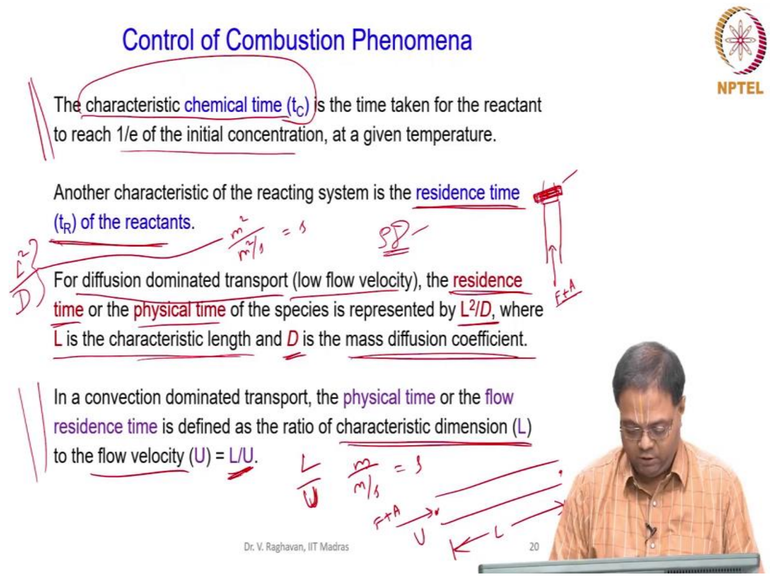

Control of Combustion Phenomena

The characteristic chemical time (t_C) is the time taken for the reactant to reach 1/e of the initial concentration, at a given temperature.

Another characteristic of the reacting system is the residence time (t_R) of the reactants.

For diffusion dominated transport (low flow velocity), the residence time or the physical time of the species is represented by L^2/D, where L is the characteristic length and D is the mass diffusion coefficient.

In a convection dominated transport, the physical time or the flow residence time is defined as the ratio of characteristic dimension (L) to the flow velocity (U) = L/U.

Now, we have already seen what is called characteristic chemical time, you have already seen this that is the initial concentration of reactants we know. So, the concentration of the reactant is reducing with time, when it reaches 1/e of its initial concentration, it takes some time to do that so that is called characteristic chemical time t_C.

The time taken by the reactant to reach 1/e of this initial concentration and a given temperature, so that will be the time of the chemical reaction the time for the chemical reaction to occur. So, we can see that so chemical time.

Then residence time is the second characteristic time we define, see for a reaction to complete it should reside within the particular space for a particular time. So, for example when the reaction should occur at a particular small control volume.

For example, I take the Bunsen burner example, so the mixture is coming out premixed here. So, now what happens here is you take a small portion in here in the exit of the Bunsen burner; if the reactants which are coming out, so there I will say fuel plus air is coming out, some premixed thing is coming out.

Now, here in this control volume it has some length scale, the control volume has some length scale. So, if the velocity of the fuel and air mixture is very high, then what happens is the time the reactant resides in this small portion is very small.

So, it resides for only a small time, but if the reaction is not able to complete within this particular small time, then reaction will not occur here; because reaction is not able to complete within the residence time of the reactant, so that is very important.

Second characteristic t_R is a residence time of the reactants. So, reactants should stay at the particular location for a given amount of time for the reaction to complete, so that is the second important characteristic time. So, how will you calculate residence time?

So, we know how you calculate the chemical time, we have seen already by using the first order and second order reaction, etcetera; we have definitions for the chemical time, so we can use that, rate of the reaction will be used to calculate the chemical time, residence time you have to calculate.

Now, there are two conditions, let us take a diffusion dominated transport, very low flow velocities, so diffusion will dominate the flow. In such a case, the residence time which is also called the physical time is defined as L^2/D, where L is the characteristic length, so as I told you some length you have to take. For example, in this case Bunsen burner it maybe diameter of the tube, some length scale or height of the flame that can be a length scale.

So, some length scale and D is the mass diffusion coefficient; so this is the time, because L^2/D will be $m^2/m^2/s$, so which is equal to second, so that will be the time scale. L^2 by the mass diffusion coefficient that is the time scale which is called residence time in a low flow velocity environment, where diffusion dominates.

So, here the diffusion coefficient is the important thing. So, when the diffusion coefficient value increases, then residence time decreases. So, when the diffusion coefficient value increases that means, the rate at which the diffusion occurs will increase, so that is ρD. If the ρD value increases, the rate of diffusion will increase.

So, the D value increases, then rate of diffusion will increase; but the residence time or the physical time will decrease. So, here similarly in the chemical time also we know that when the temperature is higher, the reaction rate is faster, chemical time will be very low.

When the reaction is infinitely fast, the chemical time will tend to 0. So, based upon the reaction rate you can see the chemical time can be smaller or larger.

In the third, convection dominated transport, you have the residence time definition as the characteristic dimension, again the characteristic dimension L and the flow velocity U. So, this will be L/U which is m/m/s equal to second, so that will be the time.

So, for example there is a combustion chamber of say length L that is the length I want to consider, some reactants are coming in, fuel plus air with the velocity of U. So, what is the time it will take for the reactant to reach from this point to the end of this, to cover the length L; what is the time? L/U, so that is the resident time; so for that time a reaction mixture will be residing in this.

If we take a small chunk, this chunk we will take, the time of L/U to travel along the length L of this, so this is the convection dominated transport, physical time or residence time is defined as the ratio of the characteristic dimension L by the flow velocity U, average flow velocity.

So, these are the time scales which we need to understand. So, chemical time scale which is dependent on the reaction rates, that is one of the time scale. So, that is actually the time from the start of the initial reaction; where the reactant concentration is going to reduce to 1/e of the initial concentration.

The residence time for a diffusive dominated transport or diffusion dominant transport will involve the dimension characteristic length or characteristic dimension and their mass diffusion coefficient. It is given by L^2/D.

On other hand, for the convection dominated flow; where the characteristic dimension is L and the flow velocity is capital U, the residence time or the physical time will be L by U. So, these are the times so chemical term t_C and the physical time or the residence time t_R, these are the two time scales which are important.