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Time and Length Scales within a Fire and Implications for Numerical Simulation

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Sheldon R. Tieszen
Sandia National Laboratories
Reactive Processes Dept. MS0836
P.O. Box 5800
Albuquerque, New Mexico, USA 87185
Fax: 505-844-8251
email:srtiesz@sandia.gov

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Abstract

A partial non-dimensionalization of the Navier-Stokes equations is used to obtain order of magnitude estimates of the rate-controlling transport processes in the reacting portion of a fire plume as a function of length scale. Over continuum length scales, buoyant time scales vary as the square root of the length scale; advection time scales vary as the length scale, and diffusion time scales vary as the square of the length scale. Due to the variation with length scale, each process is dominant over a given range. The relationship of buoyancy and baroclinc vorticity generation is highlighted. For numerical simulation, first principles solution for fire problems is not possible with foreseeable computational hardware in the near future. Filtered transport equations with subgrid modeling will be required as two to three decades of length scale are captured by solution of discretized conservation equations. By whatever filtering process one employs, one must have humble expectations for the accuracy obtainable by numerical simulation for practical fire problems that contain important multi-physics/multi-length-scale coupling with up to 10 orders of magnitude in length scale.

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Introduction

The purpose of this paper is to discuss the transport time and length scales associated with turbulent gas-phase processes in buoyant fires and to place these transport mechanisms in context of requirements for numerical simulation. In particular, this paper will focus on momentum processes and the time and length scale requirements for field modeling within the fire itself.

Extensive studies on the scaling of pool fires exist in the literature, for recent discussions, see [1-4]. The primary purpose of these studies is to quantify overall characteristics such as flame height and entrainment rate. These global characteristics are useful for engineering purposes, for inclusion into computational zone models, and to describe the far-field characteristics in field models. For the latter, it has been argued [5] that as long as the heat release of a fire is globally correct, i.e., the correct convective heat release occurs within the overall fire height (volume) then the flow external to the fire will be driven correctly. About ten cells are required across the fire diameter scaled on total heat release [5].

However, within the fire itself, global characteristics alone are not sufficient to define the extensive physical/chemical processes and their coupling. For example, Delichatsios [6] distinguishes between the scaled overall heat release, Q, which is used to define the global fire scales, and a reduced gravity, $(\Delta\rho/\rho)g$, associated with turbulent eddies. At smaller scales where combustion interactions occur, time and length scale estimates for non-premixed combustion are found in the combustion literature. Non-premixed combustion is typically defined by a time scale [7] alone, as thickness is not an intrinsic property (c.f. [8]). However, length scales can be estimated by using the Damkohler number (i.e., the ratio of a physical process time scale and a chemical time scale). If the chemical time scale and the corresponding Damkohler number are known, then by definition the time scale for the corresponding transport process is known. As will be shown in this paper, for all transport processes, there is a length scale associated with every time scale for a given process. Therefore, a length scale can be determined for the physical process that occurs over the chemical process time scale. Typically, for diffusion flames not near extinction, i.e, large Da, the length scale associated with diffusion flames in not dependent on chemistry directly, but is a balance between diffusive and advective transport processes resulting in a thickness that is dependent on the square root of the local strain rate (c.f. [8]). For fires, Cox [9] gives estimates of combustion properties in terms of velocity and length scales.

It has long been recognized within the numerical simulation community that it is not possible to capture all the relevant length scales within the fire itself with field models. Instead, filtered transport equations are used. Cox [9-10] gives details for time-filtered (Reynolds-Averaged-Navier-Stokes, or RANS) equations, the most commonly used form for fire simulations. Another form is Large Eddy Simulation, or LES, which employs a spatial-filtering technique (c.f. [11]). Implicit LES filtering, i.e., allowing the discretization scheme to determine the lower length scales, has been used in fire driven flows (c.f. [5],[12]). Once filtered, both RANS/LES equations have explicit terms representing the unresolved length and time scales that must be captured by models.

It should be obvious (but sometimes isn't), that a necessary condition for modeling a process is an understanding of it. For fires, it is necessary to understand the physical/chemical processes that contribute to the fire sustenance/spread which includes time and length scale ranges between soot production and global radiative deposition. A partial non-dimensionalization is used in the next section to review transport processes in fires, in particular buoyancy. In the interest of space, only a very cursory review of chemical processes will be given. The implications for numerical simulation follow, and concluding remarks are given.

Time and Length Scales

Time and length scales in fires are shown in Fig. 1. The smallest scales in sooty, turbulent fires that are of direct interest are those that contribute to thermal radiation, since radiative transport couples this energy back into larger length scales including fuel pyrolysis/vaporization. Soot grows from molecular length-scales O(nm) to O(100nm) in large fires (c.f. [13,14]). Since continuum approximations start at length scales on the order of O(100's nm) depending on temperature at ambient pressure [15], fundamentally, soot formation is a heterogeneous, non-continuum, chemical process. Continuum representations, such as Arrhenius-rate-equation based kinetic sets, must be considered as models for the real molecular-transport-processes.

The large end of the length scale range depends on application. For laboratory experiments, fire sizes range from O(cm to m); for building fires from O(m to 10's m); and for forest fires O(0.1km to km's). Another factor in determining the scale is if the primary interest is within the fire itself, or in the fire-induced flow which can exceed fire length scales by several orders of magnitude. For numerical simulation purposes, even if the interest is in the fire itself, often boundary conditions are set at a considerable distance O(3-10 diameters from the fire) to avoid errors [16]. Comparing the small and large scales, it can immediately be concluded that a first principles description of fires requires the coupling of some 6 to 10 or more orders of magnitude depending on the problem of interest.

The time scales involved depend on the length scales and process rates. Non-continuum transport is very rapid, due to high molecular velocities, typically on the order of 500 m/s at ambient temperature and pressure [15]. Continuum velocities on the other hand are quite low, ranging from O(0.1 mm/sec to cm/sec) at the fuel source (c.f. [17]) up to O(10's m/sec) at the top of a large O(10's m base) fire (c.f. [18]).

Continuum transport processes are expressed in terms of conservation of mass, momentum (the Navier-Stokes equations), energy and equations of state (c.f. [19]). Dimensionless numbers are obtained from non-dimensionalizing the equations (c.f. [19,20]). However, for our purposes, we wish to leave the equations in the form of a rate (1/sec) so that characteristic time scales can be identified. In this way, the transport equations can be thought of as parallel rate processes where each term represents a competing rate process. The highest rate, i.e., shortest time scale, terms are dominant. Details of the partial non-dimenionalization may be found in the appendix.

For momentum transport, the terms are:

$$\text{Buoyancy: } \tau_{ref} \sim \left(\frac{\rho_{ref}}{(\rho_{\infty} - \rho_{ref})g}\right)^{1/2} L_{ref}^{1/2}$$

$$\text{Advection: } \tau_{ref} \sim \left(\frac{1}{u_{ref}}\right) L_{ref}$$

$$\text{Diffusion: } \tau_{ref} \sim \left(\frac{1}{\nu_{ref}}\right) L_{ref}^{2}$$

Comparing these terms, it can be seen that they have different length-scale dependencies. Thus, each term dominates at a different length scale as shown in Fig. 1. At small scales, diffusion is dominant because of the high molecular-velocities relative to the bulk velocities. Representative values for viscous diffusion for air at 300 K and 2300 K are shown in Fig. 1. Molecular walk processes which define diffusion are inefficient at larger length scales and bulk advection becomes dominant. At still larger scales, buoyancy dominates. Since fire is a turbulent-mixing-limited combustion-phenomena which has a spectrum of length-scales that is driven by radiation with its own length scale spectrum from non-continuum soot emission to absorption at global application scales, all length scales play a role in this coupled multi-physics/multi-length scale problem. Therefore, while one process may dominate at a given length scale, it cannot be said that any one of these terms dominates the entire coupled process over all length scales.

The advection to diffusion ratio is the Reynolds number. In flames with fast chemistry, (Da >> 1) the balance of these forces defines the width of the diffusion flame as a function of the imposed velocity gradient across it. A two order of magnitude increase in imposed velocity will decrease the flame thickness one order of magnitude until finite rate chemistry results in extinction. This effect can be seen graphically in Fig. 1 by the noting the order of magnitude decrease in the length scale of the point of intersection between the diffusion line at the flame temperature and advective velocity lines with a two order of magnitude velocity difference. Flames are typically O(mm) depending on the imposed strain. Above this length scale, advection and buoyancy dominate transport processes.

The role of advection cannot be said to be well understood because its non-linear behavior is the source of turbulent processes with their concomitant scale changing behavior, creating the broad spectrum known as the 'turbulent cascade'. However, the role of buoyancy has received much less attention. Its role is perhaps best understood from the vorticity transport equations (curl of the Navier Stokes equations). These equations may be loosely thought of as transport equations for rotational motion, since vorticity is twice a solid body rotation rate. The gravitational (hydrostatic pressure) and local acceleration (hydrodynamic pressure) terms survive the curl operation to become explicit source terms for vorticity, as shown in the appendix. Here, both are collectively termed baroclinic vorticity generation.The local acceleration can be important relative to the gravity term when accelerations are high, as at the base of the fire [21].

An important point is that buoyancy expresses itself through vorticity generation. Since baroclinic vorticity generation is the result of a misalignment of the density gradient with the local acceleration field, it scales on this product. Therefore, vorticity will be generated at all density gradients unless they are aligned with the local acceleration field. Experimental support for this view comes from measurements that show vorticity is found at the fire edge where density gradients are located [22-23]. Vorticity will be generated at a length scale related to the density gradient length scale. Due to turbulent mixing processes in a fire, density gradients will exist across a broad spectrum of length scales from diffusive to integral scales of the turbulent eddies. Therefore, buoyancy will express itself as vorticity over the same broad length scale spectrum. Experimental evidence for this view can be found in non-reacting buoyant plume data [24] which shows a -3 spectral decay as opposed to a -5/3 spectral decay over a broad spectrum of length scales above diffusive scales. It is shown [24] that the -3 spectral decay can be obtained from scaling the ratio of buoyant and advective time scales.

It should be noted that the presence of vorticity does not imply the existence of a 'coherent vortex.' On the other hand, the existence of a vorticity source-term in the bulk flow does not automatically preclude amalgamation processes associated with vorticity transport (c.f. [25]). In other words, the large rolling motions seen at the edge of large pool fires are likely due to baroclinic vorticity generation proportional to the scale of the density gradient at the location of their generation, followed by roll-up or amalgamation [26]. Final proof of this view does not yet exist but to the author's knowledge no evidence exists to the contrary. What this picture suggests is that buoyancy expresses itself over a broad range of length and time scales that are coincident with the turbulent scale-changing processes. This view is distinctly different than the classical view that buoyancy results in linear momentum at the largest length scales followed by a turbulence cascade down to the smallest length scales.

Figure 1 shows two levels of the normalized density difference,($\Delta\rho/\rho$), of 3 and 7. The first is roughly representative of the long-time average centerline temperature (~1200°K) difference with ambient (~300°K). This gradient will exist over large length-scales in fires, since this temperature difference is relatively constant over large portions of the fire [27]. The second is related to the adiabatic flame temperature (~2300°K) and is an upper bound that exists only at small scales. The presence of a flame zone does not imply net vorticity generation at scales larger than its density gradients if the density of the fuel and air on either side are the same [28]. The total vorticity across such a flame zone is zero and serves only to accelerate the flame sheet at scales corresponding to the flame thickness (although turbulent instabilities can alias the induced velocity into larger turbulent structures).

The buoyant time scale is related to the reciprocal of the Brunt-Väisälä frequency (c.f. [29]). It can be seen in Fig. 1 for moderate velocities typical of fires, O(1-3 m/s), and a scaled density differences of 3, advection is faster, i.e., shorter time scale at a given length scale, than buoyancy up to O(10 cm) length scales. At length scales larger than O(10 cm), buoyant time scales are shorter than advection. Experimentally, it is found that fires become transitionally turbulent for O(10 cm) base diameters and are fully turbulent at O(1-3 meters) [20] consistent with the view that buoyancy expresses itself as rotational motion that becomes intertwined with turbulent processes. The ratio of the advective time scale to the buoyant time scale is the Richardson number.

Chemical time scales are dependent on temperature, composition, and specific reaction metrics (i.e., activation temperature and preexponential factors). For a given chemical time scale, comparison with the transport time scale in Fig. 1, establishes a Damkohler number. Comparison can be made to diffusive time scales or advective time scales. In general, the turbulence intensities in the small length-scale-spectrum in fires are low compared to jet flames in combustors [9] and have the appearance of wrinkled flame sheets [26]. However, long chemical times may result either from low temperatures or off-stoichiometric compositions. These conditions possibly occur in two areas in large fires. 1) In the oxygen starved, vapor dome just above the fuel source, measurements [30] indicate temperatures are on the order of 1000°K. At these conditions, kinetics calculations indicate pyrolysis reactions can occur but are fairly slow, of order tenth's of seconds [26]. Thus, it may be possible for pyrolysis to cause density gradients in the vapor domes of large fires. 2) The large rolling structures at the edge of large fires visually appear to end up filled with smoke, indicating that some form of quenching has occurred that doesn't not appear to be due to high turbulence levels. Oxygen depletion of fuel rich eddies, perhaps followed by radiative cooling, is a more reasonable hypothesis [26].

Implication to Numerical Simulation

The largest fire simulations run to date cover some two orders of magnitude in length scale [31] involving single processor machines. Using a simple scaling for uniform node spacing requires ten nodes per decade of resolved length scale. For three dimensions, this means $O(10^3)$ times the existing compute power for new every decade of resolved length scale. From Fig. 1, as a minimum, an additional factor of 10 increase in processor speed or number of processors is required to capture the shorter time scales associated with the newly resolved length scales if the computations are to be done in the advective/buoyancy controlled regime. In the diffusion controlled regime, capturing the time scales requires a factor of 100 increase for every decade resolved, and the number of transport equations increase with the number of species that exist at the short time scales. With massively parallel computing, involving $O(10^3$ to $10^4)$ processors, it can reasonable be expected that within the next several years to a decade, that an additional single decade of length scales will be resolved. Thus, perhaps 3 out of 6 to 10 decades of length scale can be resolved by discrete approximation of the conservation equations in the near future. Subgrid models consisting of engineering approximations to the closed form solutions of the conservation equations over the remaining 3 to 7 decades of length scale, that are not being integrated numerically, will be required to obtain usable solutions within a fire. While it can be argued that 'predictive' capability already exists in the engineering sense of the term, it will not exist in the scientific sense of the term until all scales are resolvable by integration of discrete approximations, or closed form solutions are found.

Figure 1 provides a useful visualization of what processes can be captured in a given length scale range. The graph can be divided into three length-scale regimes using two length-scale cut-offs. (for example, imagine vertical lines at 10 cm and 10 m in Fig. 1, capturing two orders of magnitude). Above the larger cut-off, are length scales too large to be captured and these are represented by boundary conditions in the simulation. Below the smaller cut-off, are lengths scales that have to be modeled and these are represented as source or non-linear advection terms in the transport equations. Implicit in the length scale cutoffs are time scale cutoffs corresponding to the time scales of the transport processes at the cut-off length scales.

In the author's opinion, within a fire, formal, explicit filtering of the transient equations of motion should include both spatial and temporal filtering, since the transport processes involved are linked in time and space, and small length scale processes (e.g., combustion creating density gradients creating buoyancy) are the source terms primarily responsible for driving the flow. To date this rigor has not been applied to fire problems. RANS filters the time scales explicitly but implicitly assumes that all turbulent length scales are below the filter width and are therefore modeled. Transient RANS implies that transients longer than the passage of a statistically significant number of the largest turbulent structures can be resolved. LES filters the spatial scales. However, explicit temporal filters should be applied once discrete time steps are taken. In LES, explicit filtering, not tied to the grid, should permit numerical error to be separated from modeling error as it currently does in RANS by grid refinement studies.

Filtering also formally defines the length and time scales that require modeling. Graphically in Fig. 1, modeling must be done for the region to the left of the lower cut-off (in the example given, 10 cm) for time scales below the Courant number based on the slowest velocity in the domain. The filter may be thought of as defining the volume (area) and temporal integration ranges necessary to obtain the mean value required for source (non-linear advection flux) terms in the filtered transport equations. In general, the modeled processes are nonlinear (combustion, for example) and therefore the distribution needs to be known within the integration ranges in order to capture the non-linearity. This is the principle behind PDF methods in which the product of the variable and its distribution function are taken before integration. In primitive variables, the distribution is in time and space but can be transformed into any convenient variable space as long as the transfer functions can be defined.

As an example for buoyancy, if LES calculations permitted the filter to be set at O (10 cm) resolution, then for most of the flow field in a large fire (i.e., velocities > 1 m/s), Fig. 1 suggests that buoyant processes are slower than advection processes over the modeled scales and perhaps of secondary importance as a momentum transport process in a turbulent advection closure model. All larger length scales than O (10 cm) would be resolved by the calculation. However, in a RANS calculation for the same problem, all turbulence length scales would have to be included in the model. Since it has been argued that buoyant effects are intertwined with turbulence throughout the spectrum, one would expect that buoyant 'production' of turbulence would play a significant role. While some attention has been paid to this fact [32-34], in most simulations only the effects of flow stratification have been directly addressed by buoyant production terms [35].

Conclusions

For the purposes of numerical simulation, it is useful to think of transport processes as occurring over time and length scales since these are the primitive variables over which numerical integration is taken. Partial non-dimensionalization of the transport equations is useful in identifying the rate processes for a given length scale. The buoyancy time scale varies as the square root of the length scale, advection varies linearly with length scale, and diffusion varies as the square of the length scale. Buoyancy expresses itself via baroclinic vorticity generation as rotational motion over a range of length scales from diffusional to global. As a consequence, buoyancy becomes intertwined with the turbulent cascade.

With current computational hardware, it is not possible to calculate all the relevant length and time scales to practical applications involving fire, even with the new massively parallel computers that are being developed. For the foreseeable future, filtered transport equations with subgrid modeling will be required. By whatever filtering process one employs, one must have humble expectations for the accuracy obtainable by numerical simulation with a problem that contains important multi-physics/multi-length-scale coupling with up to 10 orders of magnitude in length scale, if one can only capture two or three decades with first principles equations and the rest is modeled.

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Appendix - Reference Length and Time Scales

The Navier-Stokes equations are:

$$\frac{\partial}{\partial t}(\rho\vec{u}) + \nabla \bullet (\rho\vec{u}\vec{u}) = -\nabla P + \overrightarrow{\nabla \bullet \sigma} + (\rho - \rho_\infty)\vec{g} \quad (1)$$

For the purpose of non-dimensionalization, the following reference values are defined:

$$\vec{u}' = \vec{u}/(u_{ref}), \quad \rho' = \rho/(\rho_{ref}), \quad (\rho-\rho_\infty)' = (\rho-\rho_\infty)/(\rho_{ref}-\rho_\infty), \quad (2)$$

$$\mu' = \mu/(\mu_{ref}), \quad P' = P/(P_\infty), \quad \vec{x}' = x/(L_{ref}), \quad \nabla' = \nabla(L_{ref}), \quad t' = t/\tau_{ref}$$

The reference values can be considered as local fire plume values where τ_{ref} comparisons are being made at L_{ref} length scales.

Substituting the reference values but leaving each term as a rate, i.e, units of 1/time, gives:

$$\frac{1}{\tau_{ref}}\left[\frac{\partial}{\partial t'}(\rho'\vec{u}')\right] + \frac{u_{ref}}{L_{ref}}[\nabla' \bullet (\rho'\vec{u}'\vec{u}')] = \quad (3)$$

$$-\frac{P_\infty}{L_{ref}u_{ref}\rho_{ref}}[\nabla' P'] + \frac{\mu_{ref}}{L_{ref}^2\rho_{ref}}\overrightarrow{\nabla' \bullet \sigma'} + \frac{(\rho_{ref}-\rho_\infty)\vec{g}}{u_{ref}\rho_{ref}}[(\rho-\rho_\infty)']$$

From which one gets the following time-scale/length-scale relations:

$$\tau_{ref} \sim \left(\frac{1}{u_{ref}}\right)L_{ref} \quad \text{Advection} \qquad \tau_{ref} \sim \left(\frac{1}{\nu_{ref}}\right)L_{ref}^2 \quad \text{Diffusion} \quad (4)$$

Using the advective time scale definition gives:

$$\tau_{ref} \sim \left(\frac{\rho_{ref}}{(\rho_\infty - \rho_{ref})g}\right)^{1/2} L_{ref}^{1/2} \quad \text{Buoyancy} \quad (5)$$

Note that the same time scale definition for buoyancy comes from a similar partial non-dimensionalization of the vorticity transport equations (curl of the Navier-Stokes equations, see reference [36] for particular formulation) if the following additional reference scales are defined:

$$\omega' = \omega\tau_{ref}, \quad \nabla\rho' = \frac{L_{ref}}{(\rho_{ref}-\rho_\infty)}\nabla\rho \quad (6)$$

The result is:

$$\frac{1}{\tau_{ref}^2}\left[\frac{\partial}{\partial t'}(\vec{\omega})\right] + \frac{u_{ref}}{\tau_{ref}L_{ref}}[(\vec{u}' \bullet \nabla')\vec{\omega}' + \vec{\omega}'(\nabla' \bullet \vec{u}') - (\vec{\omega}' \bullet \nabla')\vec{u}'] = \quad (7)$$

$$\frac{u_{ref}\mu_{ref}}{L_{ref}^3\rho_{ref}}\overrightarrow{\nabla' \bullet \sigma'} + \frac{(\rho_{ref}-\rho_\infty)\vec{g}}{L_{ref}\rho_{ref}}\left[\frac{\nabla\rho'}{\rho'} \times \left(1 - \frac{u_{ref}}{\tau_{ref}g}\right)\frac{Du'}{Dt'}\right]$$

The last term is from the buoyancy term in the Navier-Stokes equations and is called the baroclinic vorticity generation term.

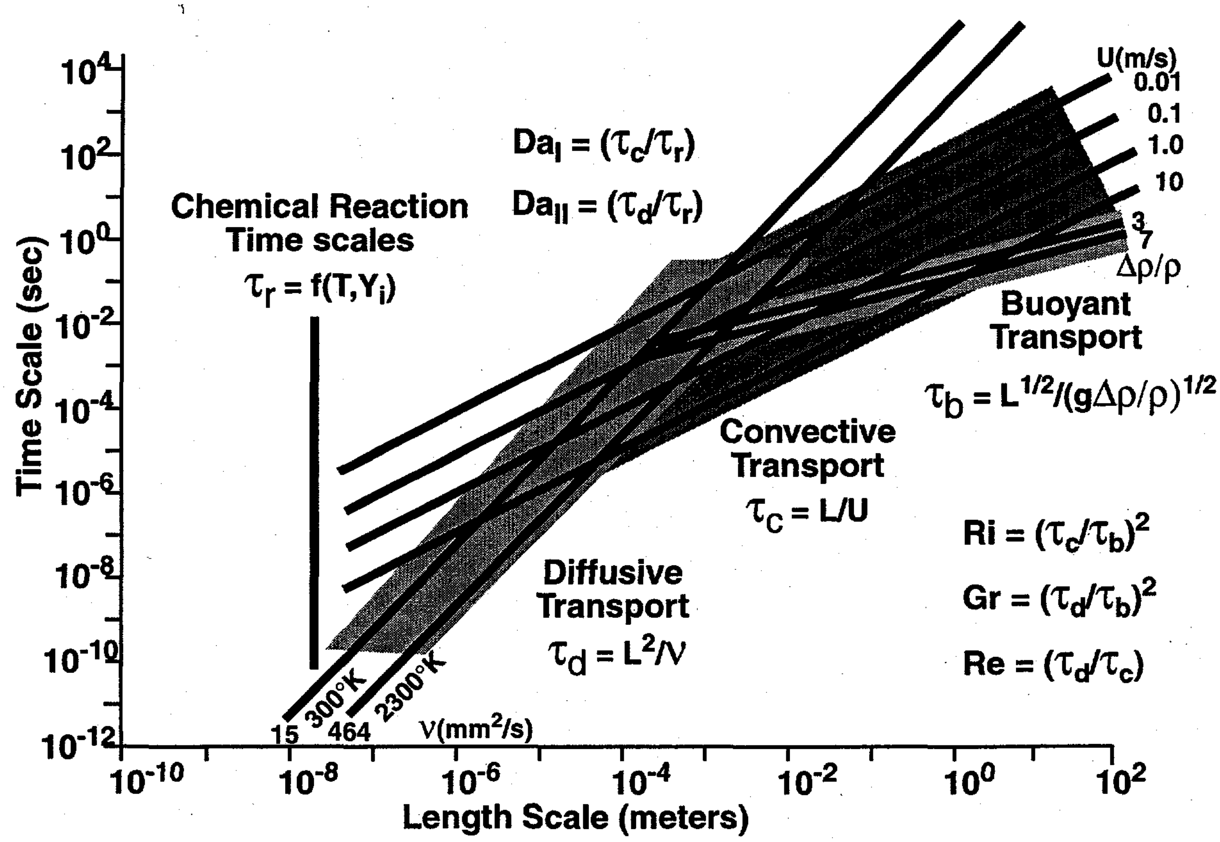

Fig. 1 - Time and Length Scales of Continuum Transport Processes Involved in Fires.