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Turbulent reacting flows

1.1 Introduction

At first glance, to the uninitiated the subject of turbulent reacting flows would appear to be relatively simple. Indeed, the basic governing principles can be reduced to a statement of conservation of chemical species and energy ((1.28), p. 16) and a statement of conservation of fluid momentum ((1.27), p. 16). However, anyone who has attempted to master this subject will tell you that it is in fact quite complicated. On the one hand, in order to understand how the fluid flow affects the chemistry, one must have an excellent understanding of turbulent flows and of turbulent mixing. On the other hand, given its paramount importance in the determination of the types and quantities of chemical species formed, an equally good understanding of chemistry is required. Even a cursory review of the literature in any of these areas will quickly reveal the complexity of the task. Indeed, given the enormous research production in these areas during the twentieth century, it would be safe to conclude that no one could simultaneously master all aspects of turbulence, mixing, and chemistry.

Notwithstanding the intellectual challenges posed by the subject, the main impetus behind the development of computational models for turbulent reacting flows has been the increasing awareness of the impact of such flows on the environment. For example, incomplete combustion of hydrocarbons in internal combustion engines is a major source of air pollution. Likewise, in the chemical process and pharmaceutical industries, inadequate control of product yields and selectivities can produce a host of undesirable byproducts. Even if such byproducts could all be successfully separated out and treated so that they are not released into the environment, the economic cost of doing so is often prohibitive. Hence, there is an ever-increasing incentive to improve industrial processes and devices in order for them to remain competitive in the marketplace.

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Given their complexity and practical importance, it should be no surprise that different approaches for dealing with turbulent reacting flows have developed over the last 50 years. On the one hand, the chemical-reaction-engineering (CRE) approach came from the application of chemical kinetics to the study of chemical reactor design. In this approach, the details of the fluid flow are of interest only in as much as they affect the product yield and selectivity of the reactor. In many cases, this effect is of secondary importance, and thus in the CRE approach greater attention has been paid to other factors that directly affect the chemistry. On the other hand, the fluid-mechanical (FM) approach developed as a natural extension of the statistical description of turbulent flows. In this approach, the emphasis has been primarily on how the fluid flow affects the rate of chemical reactions. In particular, this approach has been widely employed in the study of combustion (Rosner 1986; Peters 2000; Poinsot and Veynante 2001; Veynante and Vervisch 2002).

In hindsight, the primary factor in determining which approach is most applicable to a particular reacting flow is the characteristic time scales of the chemical reactions relative to the turbulence time scales. In the early applications of the CRE approach, the chemical time scales were larger than the turbulence time scales. In this case, one can safely ignore the details of the flow. Likewise, in early applications of the FM approach to combustion, all chemical time scales were assumed to be much smaller than the turbulence time scales. In this case, the details of the chemical kinetics are of no importance, and one is free to concentrate on how the heat released by the reactions interacts with the turbulent flow. More recently, the shortcomings of each of these approaches have become apparent when applied to systems wherein some of the chemical time scales overlap with the turbulence time scales. In this case, an accurate description of both the turbulent flow and the chemistry is required to predict product yields and selectivities accurately.

With these observations in mind, the reader may rightly ask ‘What is the approach used in this book?’ The accurate answer to this question may be ‘both’ or ‘neither,’ depending on your perspective. From a CRE perspective, the methods discussed in this book may appear to favor the FM approach. Nevertheless, many of the models find their roots in CRE, and one can argue that they have simply been rewritten in terms of detailed transport models that can be solved using computational fluid dynamics (CFD) techniques (Fox 1996a; Harris *et al*. 1996; Ranada 2002). Likewise, from an FM perspective, very little is said about the details of turbulent flows or the computational methods needed to study them. Instead, we focus on the models needed to describe the source term for chemical reactions involving *non-premixed* reactants. Moreover, for the most part, density variations in the fluid due to mixing and/or heat release are not discussed in any detail. Otherwise, the only criterion for including a particular model in this book is the requirement that it must be able to handle detailed chemistry. This criterion is motivated by the need to predict product yield and selectivity accurately for finite-rate reactions.

At first glance, the exclusion of premixed reactants and density variations might seem to be too drastic. (Especially if one equates ‘turbulent reacting flows’ with ‘combustion.’[1])

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[1] Excellent treatments of modern approaches to combustion modeling are available elsewhere (Kuznetsov and Sabel’nikov 1990; Warnatz *et al*. 1996; Peters 2000; Poinsot and Veynante 2001).

However, if one looks at the complete range of systems wherein turbulence and chemistry interact, one will find that many of the so-called ‘mixing-sensitive’ systems involve liquids or gas-phase reactions with modest density changes. For these systems, a key feature that distinguishes them from classical combusting systems is that the reaction rates are fast regardless of the temperature (e.g., acid–base chemistry). In contrast, much of the dynamical behavior of typical combusting systems is controlled by the fact that the reactants do not react at ambient temperatures. Combustion can thus be carried out in either premixed or non-premixed modes, while mixing-sensitive reactions can only be carried out in non-premixed mode. This distinction is of considerable consequence in the case of premixed combustion. Indeed, models for premixed combustion occupy a large place unto themselves in the combustion literature. On the other hand, the methods described in this book will find utility in the description of non-premixed combustion. In fact, many of them originated in this field and have already proven to be quite powerful for the modeling of diffusion flames with detailed chemistry.

In the remainder of this chapter, an overview of the CRE and FM approaches to turbulent reacting flows is provided. Because the description of turbulent flows and turbulent mixing makes liberal use of ideas from probability and statistical theory, the reader may wish to review the appropriate appendices in Pope (2000) before starting on Chapter 2. Further guidance on how to navigate the material in Chapters 2–7 is provided in Section 1.5.

1.2 Chemical-reaction-engineering approach

The CRE approach for modeling chemical reactors is based on mole and energy balances, chemical rate laws, and idealized flow models.[2] The latter are usually constructed (Wen and Fan 1975) using some combination of plug-flow reactors (PFRs) and continuous-stirred-tank reactors (CSTRs). (We review both types of reactors below.) The CRE approach thus avoids solving a detailed flow model based on the momentum balance equation. However, this simplification comes at the cost of introducing unknown model parameters to describe the flow rates between various sub-regions inside the reactor. The choice of a particular model is far from unique,[3] but can result in very different predictions for product yields with complex chemistry.

For isothermal, first-order chemical reactions, the mole balances form a system of *linear* equations. A non-ideal reactor can then be modeled as a collection of *Lagrangian* fluid elements moving *independently* through the system. When parameterized by the amount of time it has spent in the system (i.e., its residence time), each fluid element behaves as a batch reactor. The species concentrations for such a system can be completely characterized by the inlet concentrations, the chemical rate constants, and the residence time distribution (RTD) of the reactor. The latter can be found from simple tracer experiments carried out under identical flow conditions. A brief overview of RTD theory is given below.

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[2] In CRE textbooks (Hill 1977; Levenspiel 1998; Fogler 1999), the types of reactors considered in this book are referred to as *non-ideal*. The flow models must take into account fluid-mixing effects on product yields.

[3] It has been described as requiring ‘a certain amount of art’ (Fogler 1999).

For non-isothermal or non-linear chemical reactions, the RTD no longer suffices to predict the reactor outlet concentrations. From a Lagrangian perspective, local *interactions* between fluid elements become important, and thus fluid elements cannot be treated as individual batch reactors. However, an accurate description of fluid-element interactions is strongly dependent on the underlying fluid flow field. For certain types of reactors, one approach for overcoming the lack of a detailed model for the flow field is to input empirical flow correlations into so-called *zone* models. In these models, the reactor volume is decomposed into a finite collection of well mixed (i.e., CSTR) zones connected at their boundaries by molar fluxes.[4] (An example of a zone model for a stirred-tank reactor is shown in Fig. 1.5.) Within each zone, all fluid elements are assumed to be identical (i.e., have the same species concentrations). Physically, this assumption corresponds to assuming that the chemical reactions are slower than the local *micromixing time*.[5]

For non-linear chemical reactions that are fast compared with the local micromixing time, the species concentrations in fluid elements located in the same zone cannot be assumed to be identical (Toor 1962; Toor 1969; Toor and Singh 1973; Amerja *et al*. 1976). The canonical example is a non-premixed acid–base reaction for which the reaction rate constant is essentially infinite. As a result of the infinitely fast reaction, a fluid element can contain either acid or base, but not both. Due to the chemical reaction, the local fluid-element concentrations will therefore be different depending on their stoichiometric excess of acid or base. Micromixing will then determine the rate at which acid and base are transferred between fluid elements, and thus will determine the mean rate of the chemical reaction.

If all chemical reactions are fast compared with the local micromixing time, a non-premixed system can often be successfully described in terms of the *mixture fraction*.[6] The more general case of *finite-rate* reactions requires a detailed description of micromixing or, equivalently, the interactions between local fluid elements. In the CRE approach, micromixing is modeled using a Lagrangian description that follows individual fluid elements as they flow through the reactor. (Examples of micromixing models are discussed below.) A key parameter in such models is the micromixing time, which must be related to the underlying flow field.

For canonical turbulent flows (Pope 2000), the flow parameters required to complete the CRE models are readily available. However, for the complex flow fields present in most chemical reactors, the flow parameters must be found either empirically or by solving a CFD turbulence model. If the latter course is taken, the next logical step would be to attempt to reformulate the CRE model in terms of a set of transport equations that can be added to the CFD model. The principal complication encountered when following this path is the fact that the CRE models are expressed in a Lagrangian framework, whilst the CFD models are expressed in an *Eulerian* framework. One of the main goals of this book

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[4] The zones are thus essentially identical to the *finite volumes* employed in many CFD codes.
[5] The micromixing time has an exact definition in terms of the rate of decay of *concentration fluctuations*.
[6] The mixture fraction is defined in Chapter 5.

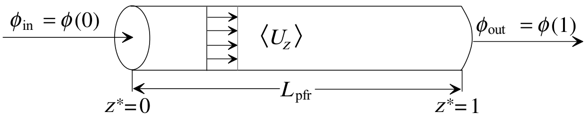

Figure 1.1. Sketch of a plug-flow reactor.

is thus to demonstrate how the two approaches can be successfully combined when both are formulated in terms of an appropriate statistical theory.

In the remainder of this section, we will review those components of the CRE approach that will be needed to understand the modeling approach described in detail in subsequent chapters. Further details on the CRE approach can be found in introductory textbooks on chemical reaction engineering (e.g., Hill 1977; Levenspiel 1998; Fogler 1999).

1.2.1 PFR and CSTR models

The PFR model is based on turbulent pipe flow in the limit where axial dispersion can be assumed to be negligible (see Fig. 1.1). The mean residence time τ_{pfr} in a PFR depends only on the mean axial fluid velocity $\langle U_z \rangle$ and the length of the reactor L_{pfr}:

$$\tau_{pfr} \equiv \frac{L_{pfr}}{\langle U_z \rangle}. \tag{1.1}$$

Defining the dimensionless axial position by $z^* \equiv z/L_{pfr}$, the PFR model for the species concentrations ϕ becomes[7]

$$\frac{d\phi}{dz^*} = \tau_{pfr}\mathbf{S}(\phi) \quad \text{with} \quad \phi(0) = \phi_{in} = \text{inlet concentrations}, \tag{1.2}$$

where $\mathbf{S}$ is the *chemical source term*. Given the inlet concentrations and the chemical source term, the PFR model is readily solved using numerical methods for initial-value problems to find the outlet concentrations $\phi(1)$.

The PFR model ignores mixing between fluid elements at *different* axial locations. It can thus be rewritten in a Lagrangian framework by substituting $\alpha = \tau_{pfr} z^*$, where α denotes the elapsed time (or *age*) that the fluid element has spent in the reactor. At the end of the PFR, all fluid elements have the same age, i.e., $\alpha = \tau_{pfr}$. Moreover, at every point in the PFR, the species concentrations are uniquely determined by the age of the fluid particles at that point through the solution to (1.2).

In addition, the PFR model assumes that mixing between fluid elements at the *same* axial location is infinitely fast. In CRE parlance, all fluid elements are said to be *well micromixed*. In a tubular reactor, this assumption implies that the inlet concentrations are uniform over the cross-section of the reactor. However, in real reactors, the inlet streams are often segregated (non-premixed) at the inlet, and a finite time is required as they move down the reactor before they become well micromixed. The PFR model can be easily

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[7] The notation is chosen to be consistent with that used in the remainder of the book. Alternative notation is employed in most CRE textbooks.

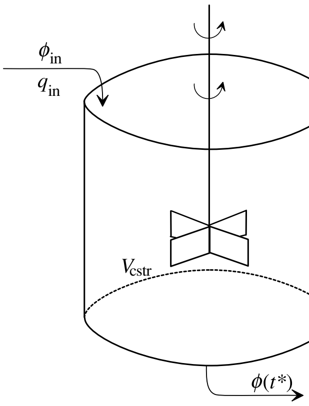

Figure 1.2. Sketch of a continuous-stirred-tank reactor (CSTR).

extended to describe radial mixing by introducing a micromixing model. We will look at a *poorly micromixed* PFR model below.

The CSTR model, on the other hand, is based on a stirred vessel with continuous inflow and outflow (see Fig. 1.2). The principal assumption made when deriving the model is that the vessel is stirred vigorously enough to eliminate all concentration gradients inside the reactor (i.e., the assumption of *well stirred*). The outlet concentrations will then be identical to the reactor concentrations, and a simple mole balance yields the CSTR model equation:

$$\frac{d\phi}{dt^*} = \tau_{cstr}\mathbf{S}(\phi) + \phi_{in} - \phi. \tag{1.3}$$

The CSTR mean residence time is defined in terms of the inlet flow rate q_{in} and the reactor volume V_{cstr} by

$$\tau_{cstr} \equiv \frac{V_{cstr}}{q_{in}}, \tag{1.4}$$

and the dimensionless time t^* is defined by $t^* \equiv t/\tau_{cstr}$. At steady state, the left-hand side of (1.3) is zero, and the CSTR model reduces to a system of (non-linear) equations that can be solved for ϕ.

The CSTR model can be derived from the fundamental scalar transport equation (1.28) by integrating the spatial variable over the entire reactor volume. This process results in an integral for the volume-average chemical source term of the form:

$$\int_{V_{cstr}} \mathbf{S}(\phi(\mathbf{x}, t))\, d\mathbf{x} = V_{cstr}\mathbf{S}(\phi(t)), \tag{1.5}$$

where the right-hand side is found by invoking the assumption that ϕ is independent of $\mathbf{x}$. In the CRE parlance, the CSTR model applies to a reactor that is both *well macromixed* and *well micromixed* (Fig. 1.3). The well macromixed part refers to the fact that a fluid element's location in a CSTR is *independent* of its age.[8] This fact follows from the well

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[8] The PFR is thus not well macromixed since a fluid element's location in a PFR is a linear function of its age.

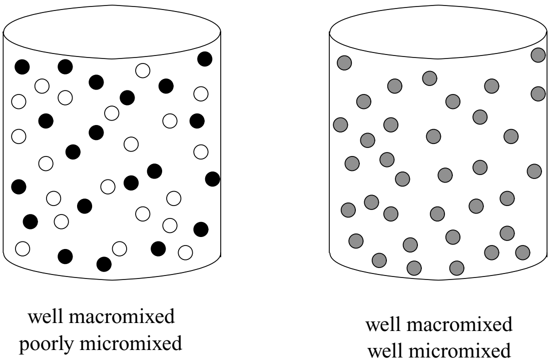

Figure 1.3. Sketch of a poorly micromixed versus a well micromixed CSTR.

stirred assumption, but is not equivalent to it. Indeed, if fluid elements inside the reactor did not interact due to micromixing, then the fluid concentrations ϕ would depend only on the age of the fluid element. Thus, the CSTR model also implies that the reactor is well micromixed.[9] We will look at the extension of the CSTR model to well macromixed but poorly micromixed systems below.

The applicability of the PFR and CSTR models for a particular set of chemical reactions depends on the characteristic time scales of reaction rates relative to the mixing times. In the PFR model, the only relevant mixing times are the ones that characterize radial dispersion and micromixing. The former will be proportional to the integral time scale of the turbulent flow,[10] and the latter will depend on the inlet flow conditions but, at worst, will also be proportional to the turbulence integral time scale. Thus, the PFR model will be applicable to chemical reaction schemes[11] wherein the shortest chemical time scale is greater than or equal to the turbulence integral time scale.

On the other hand, for the CSTR model, the largest time scale for the flow will usually be the *recirculation time*.[12] Typically, the recirculation time will be larger than the largest turbulence integral time scale in the reactor, but smaller than the mean residence time. Chemical reactions with characteristic time scales larger than the recirculation time can be successfully treated using the CSTR model. Chemical reactions that have time scales intermediate between the turbulence integral time scale and the recirculation time should be treated by a CSTR zone model. Finally, chemical reactions that have time scales smaller than the turbulence integral time scale should be described by a micromixing model.

[9] In the statistical theory of fluid mixing presented in Chapter 3, well macromixed corresponds to the condition that the scalar means $\langle \phi \rangle$ are independent of position, and well micromixed corresponds to the condition that the scalar variances are null. An equivalent definition can be developed from the residence time distribution discussed below.

[10] In Chapter 2, we show that the turbulence integral time scale can be defined in terms of the turbulent kinetic energy k and the turbulent dissipation rate ε by $\tau_u = k/\varepsilon$. In a PFR, τ_u is proportional to $D/\langle U_z \rangle$, where D is the tube diameter.

[11] The chemical time scales are defined in Chapter 5. In general, they will be functions of the temperature, pressure, and local concentrations.

[12] Heuristically, the recirculation time is the average time required for a fluid element to return to the impeller region after leaving it.

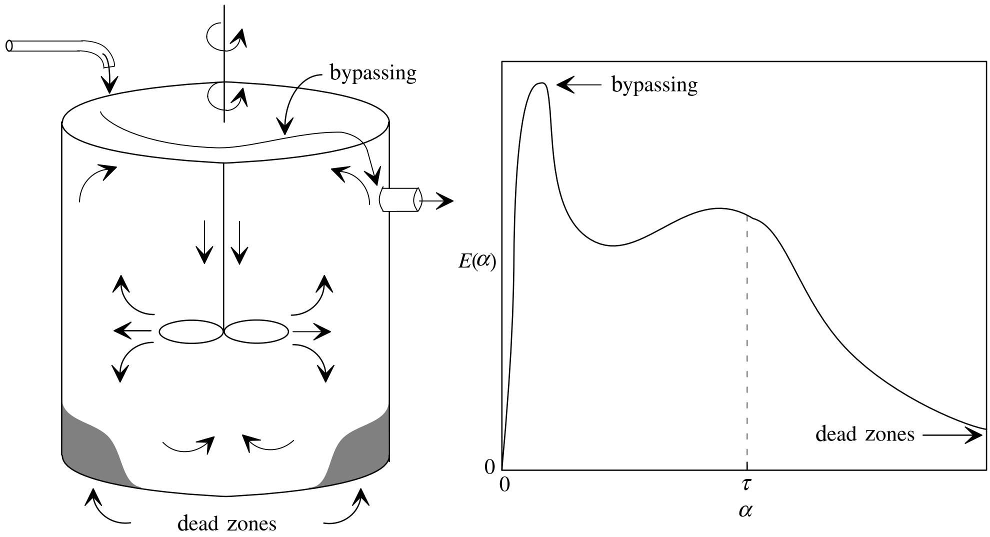

Figure 1.4. Sketch of the residence time distribution (RTD) in a non-ideal reactor.

1.2.2 RTD theory

In the CRE literature, the residence time distribution (RTD) has been shown to be a powerful tool for handling isothermal first-order reactions in arbitrary reactor geometries. (See Nauman and Buffham (1983) for a detailed introduction to RTD theory.) The basic ideas behind RTD theory can be most easily understood in a Lagrangian framework. The residence time of a fluid element is defined to be its age α as it leaves the reactor. Thus, in a PFR, the *RTD function* $E(\alpha)$ has the simple form of a delta function:

$$E_{\text{pfr}}(\alpha) = \delta(\alpha - \tau_{\text{pfr}}), \tag{1.6}$$

i.e., all fluid elements have identical residence times. On the other hand, in a CSTR, the RTD function has an exponential form:[13]

$$E_{\text{cstr}}(\alpha) = \frac{1}{\tau_{\text{cstr}}} \exp\left(-\frac{\alpha}{\tau_{\text{cstr}}}\right). \tag{1.7}$$

RTD functions for combinations of ideal reactors can be constructed (Wen and Fan 1975) based on (1.6) and (1.7). For non-ideal reactors, the RTD function (see example in Fig. 1.4) can be measured experimentally using passive tracers (Levenspiel 1998; Fogler 1999), or extracted numerically from CFD simulations of time-dependent passive scalar mixing.

In this book, an alternative description based on the *joint probability density function* (PDF) of the species concentrations will be developed. (Exact definitions of the joint PDF and related quantities are given in Chapter 3.) The RTD function is in fact the PDF of the fluid-element ages as they leave the reactor. The relationship between the PDF description and the RTD function can be made transparent by defining a fictitious chemical species

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[13] The outflow of a CSTR is a *Poisson process*, i.e., fluid elements are randomly selected regardless of their position in the reactor. The *waiting time* before selection for a Poisson process has an exponential probability distribution. See Feller (1971) for details.

ϕ_τ whose inlet concentration is null, and whose chemical source term is $S_\tau = 1$. Owing to turbulent mixing in a chemical reactor, the PDF of ϕ_τ will be a function of the *composition-space variable* ψ, the spatial location in the reactor $\mathbf{x}$, and time t. Thus, we will denote the PDF by $f_\tau(\alpha; \mathbf{x}, t)$. The PDF of ϕ_τ *at the reactor outlet*, $\mathbf{x}_{\text{outlet}}$, is then equal to the *time-dependent* RTD function:

$$E(\alpha, t) = f_\tau(\alpha; \mathbf{x}_{\text{outlet}}, t). \tag{1.8}$$

At steady state, the PDF (and thus the RTD function) will be independent of time. Moreover, the *internal-age distribution* at a point $\mathbf{x}$ inside the reactor is just $I(\alpha; \mathbf{x}, t) = f_\tau(\alpha; \mathbf{x}, t)$. For a *statistically homogeneous* reactor (i.e., a CSTR), the PDF is independent of position, and hence the steady-state internal-age distribution $I(\alpha)$ will be independent of time and position.

One of the early successes of the CRE approach was to show that RTD theory suffices to treat the special case of *non-interacting* fluid elements (Danckwerts 1958). For this case, each fluid element behaves as a *batch reactor*:

$$\frac{\mathrm{d}\boldsymbol{\phi}_{\text{batch}}}{\mathrm{d}\alpha} = \mathbf{S}(\boldsymbol{\phi}_{\text{batch}}) \quad \text{with} \quad \boldsymbol{\phi}_{\text{batch}}(0) = \boldsymbol{\phi}_{\text{in}}. \tag{1.9}$$

For fixed initial conditions, the solution to this expression is uniquely defined in terms of the age, i.e., $\boldsymbol{\phi}_{\text{batch}}(\alpha)$. The *joint composition PDF* $f_{\boldsymbol{\phi}}(\boldsymbol{\psi}; \mathbf{x}, t)$ *at the reactor outlet* is then uniquely defined in terms of the time-dependent RTD distribution:[14]

$$f_{\boldsymbol{\phi}}(\boldsymbol{\psi}; \mathbf{x}_{\text{outlet}}, t) = \int_0^\infty \delta(\boldsymbol{\psi} - \boldsymbol{\phi}_{\text{batch}}(\alpha)) E(\alpha, t)\,\mathrm{d}\alpha, \tag{1.10}$$

where the multi-variable delta function is defined in terms of the product of single-variable delta functions for each chemical species by

$$\boldsymbol{\delta}(\boldsymbol{\psi} - \boldsymbol{\phi}) \equiv \prod_\beta \delta(\psi_\beta - \phi_\beta). \tag{1.11}$$

For the general case of *interacting* fluid elements, (1.9) and (1.10) no longer hold. Indeed, the correspondence between the RTD function and the composition PDF breaks down because the species concentrations inside each fluid element can no longer be uniquely parameterized in terms of the fluid element's age. Thus, for the general case of complex chemistry in non-ideal reactors, a mixing theory based on the composition PDF will be more powerful than one based on RTD theory.

The utility of RTD theory is best illustrated by its treatment of *first-order* chemical reactions. For this case, each fluid element can be treated as a batch reactor.[15] The concentration

[14] At steady state, the left-hand side of this expression has independent variables $\boldsymbol{\psi}$. For fixed $\boldsymbol{\psi} = \boldsymbol{\psi}^*$, the integral on the right-hand side sweeps over all fluid elements in search of those whose concentrations $\boldsymbol{\phi}_{\text{batch}}$ are equal to $\boldsymbol{\psi}^*$. If these fluid elements have the same age (say, $\alpha = \alpha^*$), then the joint PDF reduces to $f_{\boldsymbol{\phi}}(\boldsymbol{\psi}^*; \mathbf{x}_{\text{outlet}}) = E(\alpha^*)$, where $E(\alpha^*)\,\mathrm{d}\alpha^*$ is the fraction of fluid elements with age α^*.

[15] Because the outlet concentrations will not depend on it, micromixing between fluid particles can be neglected. The reader can verify this statement by showing that the micromixing term in the poorly micromixed CSTR and the poorly micromixed PFR falls out when the mean outlet concentration is computed for a first-order chemical reaction. More generally, one can show that the chemical source term appears in closed form in the transport equation for the scalar means.

of a chemical species in a fluid element then depends only on its age through the solution to the batch-reactor model:

$$\frac{\mathrm{d}\phi}{\mathrm{d}\alpha} = -k\phi \quad \text{with} \quad \phi(0) = \phi_{\text{in}}, \tag{1.12}$$

i.e.,

$$\phi(\alpha) = \phi_{\text{in}} \mathrm{e}^{-k\alpha}. \tag{1.13}$$

In RTD theory, the concentrations at the reactor outlet are found by averaging over the ages of all fluid elements leaving the reactor:[16]

$$\phi_{\text{out}} = \int_0^\infty \phi(\alpha) E(\alpha)\, \mathrm{d}\alpha. \tag{1.14}$$

Thus, for first-order reactions, exact solutions can be found for the outlet concentration, e.g., from (1.13):

$$\left(\frac{\phi_{\text{out}}}{\phi_{\text{in}}}\right)_{\text{pfr}} = \mathrm{e}^{-k\tau_{\text{pfr}}} \quad \text{and} \quad \left(\frac{\phi_{\text{out}}}{\phi_{\text{in}}}\right)_{\text{cstr}} = \frac{1}{1 + k\tau_{\text{cstr}}}.$$

For higher-order reactions, the fluid-element concentrations no longer obey (1.9). Additional terms must be added to (1.9) in order to account for micromixing (i.e., local fluid-element interactions due to molecular diffusion). For the poorly micromixed PFR and the poorly micromixed CSTR, extensions of (1.9) can be employed with (1.14) to predict the outlet concentrations in the framework of RTD theory. For non-ideal reactors, extensions of RTD theory to model micromixing have been proposed in the CRE literature. (We will review some of these micromixing models below.) However, due to the non-uniqueness between a fluid element's concentrations and its age, micromixing models based on RTD theory are generally *ad hoc* and difficult to validate experimentally.

1.2.3 Zone models

An alternative method to RTD theory for treating non-ideal reactors is the use of zone models. In this approach, the reactor volume is broken down into well mixed zones (see the example in Fig. 1.5). Unlike RTD theory, zone models employ an Eulerian framework that ignores the age distribution of fluid elements inside each zone. Thus, zone models ignore micromixing, but provide a model for macromixing or large-scale inhomogeneity inside the reactor.

Denoting the *transport rate* of fluid from zone i to zone j by f_{ij}, a zone model can be expressed mathematically in terms of mole balances for each of the N zones:

$$\frac{\mathrm{d}\phi^{(i)}}{\mathrm{d}t} = \sum_{j=0}^{N+1} \left(f_{ji}\phi^{(j)} - f_{ij}\phi^{(i)} \right) + \mathbf{S}\left(\phi^{(i)}\right) \quad i = 1, \dots, N. \tag{1.15}$$

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[16] For non-interacting fluid elements, the RTD function is thus equivalent to the joint PDF of the concentrations. In composition space, the joint PDF would lie on a one-dimensional sub-manifold (i.e., have a one-dimensional support) parameterized by the age α. The addition of micromixing (i.e., interactions between fluid elements) will cause the joint PDF to spread in composition space, thereby losing its one-dimensional support.