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Some Analytic Solutions for Stochastic Reactor Models Based on the Joint Composition PDF

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Abstract

The stochastic reactor models Partially Stirred Reactor (PaSR) and Partially Stirred Plug Flow Reactor (PaSPFR) have been investigated. These models are based on a simplified joint composition PDF transport equation. Analytic solutions for five different Cauchy problems for the PDF transport equation as given by the stochastic reactor models are presented. In all cases, molecular mixing in the stochastic reactor models is described by the LMSE mixing model. The analytic solutions have been found by combining the method of characteristics with a set of ordinary differential equations for the statistical moments to account for the functional dependence of the coefficients in the corresponding PDF transport equation. For each case an example problem is discussed to illustrate the behavior of the analytic solution.

Contents

1 Introduction

Stochastic reactor models (SRMs) like the partially stirred reactor (PaSR) and partially stirred plug flow reactor (PaSPFR) have been recently applied to investigate a variety of combustion related problems. These models account for micromixing effects while they are computationally feasible for chemical systems with a large number of chemical species and many chemical reactions. Therefore, SRMs are particularly suited to study pollutant formation in combustion devices. Curl [1] introduced a random dispersion model that can be regarded as one of the first SRMs. This model has been applied in conjunction with a simple chemical mechanism to simulate NOx formation [2]. More recently, Correa [3] used the PaSR model with a detailed chemical mechanism to study the turbulence-chemistry interaction. Several chemical systems have been investigated using SRMs. NO formation has been studied in a gas turbine environment in cases of both premixed [4] and nonpremixed [5] combustion systems. Another field in which SRMs have been applied is in the incineration of hazardous waste whereby the influence of turbulence mixing on the combustion of chlorinated hydrocarbons has been studied [6, 7]. SRMs have also been used to investigate differences between molecular mixing models. In [8] and [9] a computational study is presented in which different mixing models have been compared with each other. Another field of application for SRMs is the validation of simplified chemistry models because simplified and detailed chemistry models can both be compared in a range of Damköhler numbers that is relevant for turbulent combustion. In [10] a global step reaction has been fitted to describe nonpremixed CO oxidation for a certain range of turbulent time scales. In [11] and [12] systematically reduced chemical mechanisms for CO and NO chemistry have been validated for several degrees of turbulent mixing. SRMs have also been applied to investigate numerical properties that are important for the numerical treatment of more complicated equations. For example, the accuracy of operator splitting has been investigated employing the PaSR model [13]. In [11] a new algorithm for the PaSR has been developed that eliminates time step dependence.

While the work mentioned thus far has been purely computational, SRMs have been also used to model real combustion devices. In [14], soot formation in a diesel engine was modeled using a SRM which included a detailed model for soot formation combined with a reduced gas phase mechanism. In [15], an experimental and a computational study of the influence of turbulence intensity on the formation of products of incomplete combustion in a stationary turbulent flow reactor has been presented. Good agreement between experiments and simulation results has been achieved. In [16] the same reactor has been studied but a more detailed gas phase model and a detailed model for the formation of soot has been implemented in the PaSPFR model.

Both SRMs can be rigorously derived from the one-point joint scalar PDF transport equation [17] as demonstrated in [18] by assuming statistical homogeneity. The resulting equation contains a term for the chemical reactions and the molecular mixing in case of the PaSPFR and an additional in and outflow term in case of the PaSR model. As in the case of the full PDF transport equation, the term that describes the micromixing has to be modeled. The random dispersion model introduced by Curl is just one out of many known mixing models. In the most general case, the SRMs are given by the following integro-differential equation that describes the evolution of the joint composition mass density function (MDF):

$$\begin{aligned}\frac{\partial \mathcal{F}(\underline{\psi};t)}{\partial t} &+ \underbrace{\sum_{k=1}^{K+1} \frac{\partial}{\partial \psi_k}(A_k \mathcal{F}(\underline{\psi};t))}_{O_1} - \underbrace{\frac{1}{2}\sum_{k,l=1}^{K+1} \frac{\partial^2}{\partial \psi_k \partial \psi_l}(B_{kl}\mathcal{F}(\underline{\psi};t))}_{O_2} \\ &- \underbrace{\int W(\underline{\psi}|\underline{\psi_a};t)\mathcal{F}(\underline{\psi_a};t) - W(\underline{\psi_a}|\underline{\psi};t)\mathcal{F}(\underline{\psi};t)d\underline{\psi_a}}_{O_3} \\ &= \underbrace{\frac{1}{\tau_{PaSR}}\left(\mathcal{F}_{in}(\underline{\psi}) - \mathcal{F}(\underline{\psi};t)\right)}_{O_4}. \qquad (1)\end{aligned}$$

starting from some initial condition:

$$\mathcal{F}(\underline{\psi};0) = \mathcal{F}_0(\underline{\psi}). \qquad (2)$$

Equation (1) describes the PaSR model. Without the inhomogeneity, i.e. if O_4 is zero, equation (1) describes the PaSPFR model. It is a first order quasi-linear partial differential equation. Equation (1), with an initial condition (2), represents a Cauchy problem. The residence time in the PaSR is denoted as τ_{PaSR}. The sample variable, ψ_k, represents the realization of the random variable, ϕ_k. Scalar variables are bounded, and therefore the MDF, $\mathcal{F}(\underline{\psi};t)$, at any time, $t \in [0,\infty)$, can be assumed to have compact support.

The different operators represent different models for micromixing and chemical reaction. The operator O_1 describes a drift in compositions space. The deterministic mixing model LMSE (also called IEM model) has this form. This operator also describes the change of the MDF in composition space due to chemical reactions. Other mixing models like the binomial Langevin mixing model [19] are given by a combination of the operators O_1 and O_2 . Mixing models that belong to the group of coalescence dispersion models, like the CURL model, are described by operator O_3. For a typical combustion problem, equation (1) has the following properties:

- The joint composition MDF has a *high dimension.* Detailed chemistry models can contain up to 100 chemical species and 1000 elementary reactions.

- The chemical source term in equation (1) is highly *nonlinear* and couples different species and temperature. Due to different time scales inherent in the set of elementary reactions, the resulting operator is usually *stiff.*

- The coefficients for some mixing models depend on functionals of the MDF, i.e. they contain *statistical moments* as the mean or the variance.

- The PaSR-model transport equation is *inhomogeneous*.

In this paper we focus on the LMSE-mixing model. The coefficients of equation (1) are set to:

$$\begin{aligned} A_k(\underline{\psi}, \underline{\widetilde{\phi}}) &= -\frac{1}{2}\frac{C_\phi}{\tau}(\psi_k - \widetilde{\phi_k}) + S_k \\ B_{kl} &= 0 \\ W(\underline{\psi}|\underline{\psi_a}; t) = W(\underline{\psi_a}|\underline{\psi}; t) &= 0. \end{aligned} \tag{3}$$

In the following, we call equation (1) with coefficients (3) PaSPFR-LMSE or PaSR-LMSE, depending on whether we look at the homogeneous or inhomogeneous equation. The factor C_ϕ represents a model constant that is usually of order unity and τ denotes the mixing time. Besides the chemical source term S_k, the coefficient A_k contains the scalar Favre mean $\widetilde{\phi_k}$. It is defined as:

$$\widetilde{\phi_k} \quad = \quad \frac{\int_{-\infty}^{\infty} \psi_k \mathcal{F}(\underline{\psi}; t) d\underline{\psi}}{\int_{-\infty}^{\infty} \mathcal{F}(\underline{\psi}; t) d\underline{\psi}}. \tag{4}$$

Therefore, the coefficient vector $(A_k)_{k=1,\dots,K+1}$, as defined by equation (3), depends on the Favre mean and, as a consequence on the MDF itself.

To obtain a solution for the Cauchy problem (1) and (2) a numerical method is needed to account for the special features described earlier. The high dimension of the function $\mathcal{F}$ requires that a finite difference or a finite element method must be highly adaptive to the solution to reduce storage and time cost. For a low dimensional $\mathcal{F}$, an adaptive Galerkin method using moving weights as a prefactor to orthogonal polynomials has been developed [20]. Nevertheless, an extension of this numerical method to higher dimensions is not straightforward if possible at all [21]. Alternatively, particle methods can be used. The complexity of particle methods increases only linearly with the dimension of $\mathcal{F}$ at the expense of a high approximation error between the set of particles and $\mathcal{F}$ [17]. The different character of the operators in (1) motivate the application of an operator splitting technique. Operator splitting techniques are used to split evolution equations into simpler problems. The common advantage of all splittings is the possibility to solve the splitted equations independently with different numerical schemes. The accuracy of operator splitting, the numerical approximation of the splitted operator, and the particle method is an important issue in order to determine whether one can rely on the numerical solution. In [17] numerical experiments have been performed to estimate the order of convergence for different splitting schemes. If there were an analytic solution available then we could not only give the order of convergence but we could also determine the absolute size of the numerical error as distinguishing between the contributions of error coming from the different approximations. One purpose of this paper is to present an analytic solution for simple cases of the Cauchy problem (1) and (2). These analytic solutions can then be used for different purposes. They provide insight in each term appearing in the SRM equations. They can be used to investigate the approximation error of numerical schemes [22]. Moreover, it is possible to use these analytical solutions for a simple case to construct a new numerical scheme [18, 22]. Another purpose of this paper is to present the technique to obtain analytic solutions of the Cauchy problem (1) and (2) for these simple cases. Equation (1) represents a first order quasi-linear partial differential equation. Due to the functional dependence of the coefficients A_k the method of characteristics can not be applied in a straightforward manner. In the next section a technique is presented that uses the method of characteristics as well as ordinary differential equations for the moments of $\mathcal{F}$.

In the following we present the analytic solutions of five cases. The first case is the PaSPFR-LMSE assuming there are no chemical reactions and mixing only. A slightly more complex case follows in which a first order chemical reaction and mixing are analyzed simultaneously. For the PaSR-LMSE reactor model, we examine three different cases. The PaSR model only with an inflow and outflow without mixing and reaction is studied first. This analytic solution has been used in [18] to construct a time step independent particle algorithm for the PaSR. Second, the PaSR with mixing is studied and third the analytic solution to the full PaSR equation, including inflow and outflow, a first order reaction, and mixing is presented.

2 PaSPFR-LMSE, No Reaction

In order to demonstrate the solution technique we start with the most simple case. The PaSPFR-LMSE model for one inert species. First, we show how to find the solution, then we state a theorem, and finally proof the assertion made. Consider the following Cauchy problem

$$\frac{\partial \mathcal{F}(\psi;t)}{\partial t} = \frac{1}{2}\frac{C_\phi}{\tau}\frac{\partial}{\partial \psi}\left((\psi-\tilde{\phi})\mathcal{F}(\psi;t)\right) \tag{5}$$

$$\mathcal{F}(\psi;0) = \mathcal{F}_0(\psi) \tag{6}$$

and assume that at any time $t \in [0,\infty)$ the MDF $\mathcal{F}(\psi;t)$ has compact support in ψ. The dependence of the coefficients on $\tilde{\phi}$ can be removed by solving a system of ordinary differential equations for the moments that are functionals of $\mathcal{F}(\psi;t)$. The idea is to substitute the integral terms in the Favre average by two functions $a(t), b(t)$, i.e. the total mass and the mean mass fraction of ϕ. Then the time evolution of this functions is calculated and fed into the partial differential equation. The resulting PDE is solved by the method of characteristics. Derive right hand side of equation (5)

$$\begin{aligned}\frac{\partial \mathcal{F}(\psi;t)}{\partial t} &= \frac{1}{2}\frac{C_\phi}{\tau}\frac{\partial}{\partial \psi}\left((\psi-\tilde{\phi})\mathcal{F}(\psi;t)\right)\\ &= \frac{1}{2}\frac{C_\phi}{\tau}\mathcal{F}(\psi;t)+\left(\frac{1}{2}\frac{C_\phi}{\tau}\psi-\frac{1}{2}\frac{C_\phi}{\tau}\tilde{\phi}\right)\frac{\partial}{\partial \psi}\mathcal{F}(\psi;t)\end{aligned}$$

Substitute the term for the Favre average $\tilde{\phi}$

$$\frac{b(t)}{a(t)} := \tilde{\phi} = \frac{\int_{-\infty}^{\infty}\psi\mathcal{F}(\psi;t)d\psi}{\int_{-\infty}^{\infty}\mathcal{F}(\psi;t)d\psi}$$

Calculate time evolution of $b(t), a(t)$

$$\begin{aligned}b(t) &= \int_{-\infty}^{\infty}\psi\mathcal{F}(\psi;t)d\psi\\ \frac{d}{dt}b(t) &= \frac{d}{dt}\int_{-\infty}^{\infty}\psi\mathcal{F}(\psi;t)d\psi\\ &= \int_{-\infty}^{\infty}\psi\frac{\partial}{\partial t}\mathcal{F}(\psi;t)d\psi\end{aligned}$$

Replace $\frac{\partial}{\partial t}\mathcal{F}(\psi;t)$ by the right hand side of the evolution equation (5).

$$\begin{aligned}\frac{d}{dt}b(t) &= \int_{-\infty}^{\infty}\psi\left(\frac{1}{2}\frac{C_\phi}{\tau}\mathcal{F}(\psi;t)+\left(\frac{1}{2}\frac{C_\phi}{\tau}\psi-\frac{1}{2}\frac{C_\phi}{\tau}\frac{b(t)}{a(t)}\right)\frac{\partial}{\partial\psi}\mathcal{F}(\psi;t)\right)d\psi\\ &= \frac{1}{2}\frac{C_\phi}{\tau}\left(\int_{-\infty}^{\infty}\psi\left(\mathcal{F}(\psi;t)+\psi\frac{\partial}{\partial\psi}\mathcal{F}(\psi;t)-\frac{b(t)}{a(t)}\frac{\partial}{\partial\psi}\mathcal{F}(\psi;t)\right)d\psi\right)\\ &= \frac{1}{2}\frac{C_\phi}{\tau}\left(b(t)+\left[\psi^2\mathcal{F}(\psi;t)\mid_{-\infty}^{\infty} -2\int_{-\infty}^{\infty}\psi\mathcal{F}(\psi;t)d\psi\right]\right.\\ &\quad\left.-\frac{b(t)}{a(t)}\left[\psi\mathcal{F}(\psi;t)\mid_{-\infty}^{\infty}-\int_{-\infty}^{\infty}\mathcal{F}(\psi;t)d\psi\right]\right)\\ &= \frac{1}{2}\frac{C_\phi}{\tau}\left(b(t)-2b(t)+b(t)\right)\\ &= 0\end{aligned}$$

It follows that $b(t) = const. = b_0 = \int_R \psi\mathcal{F}_0(\psi)d\psi$. Analogously we have for $a(t)$

$$\begin{aligned}a(t) &= \int_{-\infty}^{\infty}\mathcal{F}(\psi;t)d\psi\\ \frac{d}{dt}a(t) &= \frac{d}{dt}\int_{-\infty}^{\infty}\mathcal{F}(\psi;t)d\psi\\ &= \frac{1}{2}\frac{C_\phi}{\tau}\int_{-\infty}^{\infty}\frac{\partial}{\partial t}\mathcal{F}(\psi;t)d\psi\\ &= \int_{-\infty}^{\infty}\mathcal{F}(\psi;t)d\psi+\int_{-\infty}^{\infty}\psi\frac{\partial}{\partial\psi}\mathcal{F}(\psi;t)d\psi-\frac{b(t)}{a(t)}\int_{-\infty}^{\infty}\frac{\partial}{\partial\psi}\mathcal{F}(\psi;t)d\psi\\ &= 0.\end{aligned}$$

Therefore, $a(t) = a_0$ is also constant in time. The characteristic equations are then given as:

$$\begin{aligned}
\frac{d}{dt}\psi &= -\frac{C_\phi}{2\tau}\left(\psi - \frac{b_0}{a_0}\right) && \psi(0) = \psi_0 \\
\frac{d}{dt}\mathcal{F} &= \frac{C_\phi}{2\tau}\mathcal{F} && \mathcal{F}(0) = \mathcal{F}_0.
\end{aligned}$$

The corresponding inverse characteristic curve is given by

$$\psi^*(t) = \frac{b_0}{a_0} - \frac{b_0}{a_0}\exp[\frac{C_\phi}{2\tau}t] + \psi\exp[\frac{C_\phi}{2\tau}t]$$

and we can write the solution as

$$\mathcal{F}(\psi;t) = \mathcal{F}_0(\psi^*(t))\exp[\frac{C_\phi}{2\tau}t].$$

Theorem 1 *Let the initial function $\mathcal{F}_0(\psi)$ be sufficiently smooth and assume that at any time $t \in [0,\infty)$ the MDF $\mathcal{F}(\psi;t)$ has compact support in ψ. Then, the analytic solution for equation (5) is given by*

$$\mathcal{F}(\psi;t) = \mathcal{F}_0\left(\psi\,\exp(\frac{C_\phi}{2\tau}t) + \frac{b_0}{a_0}(1 - \exp(\frac{C_\phi}{2\tau}t))\right)\exp(\frac{C_\phi}{2\tau}t) \tag{7}$$

with

$$a_0 = \int_{-\infty}^{\infty}\mathcal{F}_0(\psi)d\psi \tag{8}$$

$$b_0 = \int_{-\infty}^{\infty}\psi\mathcal{F}_0(\psi)d\psi. \tag{9}$$

Proof : This solution is validated by calculating the different terms in the transport equation and combining them zero. First, we calculate the t-derivative of the solution.

$$\begin{aligned}
\frac{\partial}{\partial t}\mathcal{F} &= \frac{\partial}{\partial t}\left[\mathcal{F}_0(\psi^*(t))\exp[\frac{C_\phi}{2\tau}t]\right] \\
&= \mathcal{F}_0(\psi^*(t))\frac{\partial}{\partial t}\exp[\frac{C_\phi}{2\tau}t] + \exp[\frac{C_\phi}{2\tau}t]\frac{\partial}{\partial t}\mathcal{F}_0(\psi^*(t)) \\
&= \exp[\frac{C_\phi}{2\tau}t]\mathcal{F}_0'(\psi^*(t)) \times \left[\psi\frac{C_\phi}{2\tau}\exp[\frac{C_\phi}{2\tau}t] - \frac{b_0}{a_0}\frac{C_\phi}{2\tau}\exp[\frac{C_\phi}{2\tau}t]\right] \\
&\quad + \frac{C_\phi}{2\tau}\mathcal{F}_0(\psi^*(t))\exp[\frac{C_\phi}{2\tau}t] \\
&= \frac{C_\phi}{2\tau}\mathcal{F}_0(\psi^*(t))\exp[\frac{C_\phi}{2\tau}t] + \psi\frac{C_\phi}{2\tau}\mathcal{F}_0'(\psi^*(t))\exp[\frac{C_\phi}{\tau}t] \\
&\quad - \frac{b_0}{a_0}\frac{C_\phi}{2\tau}\mathcal{F}_0'(\psi^*(t))\exp[\frac{C_\phi}{\tau}t]
\end{aligned}$$

Then, we calculate ψ-derivative of solution.

$$\begin{aligned}
\frac{\partial}{\partial\psi}\mathcal{F}(\psi;t) &= \frac{\partial}{\partial\psi}\mathcal{F}_0(\psi^*(t))\exp[\frac{C_\phi}{2\tau}t] \\
&= \exp[\frac{C_\phi}{2\tau}t]\frac{\partial}{\partial\psi}\mathcal{F}_0(\psi^*(t)) \\
&= \exp[\frac{C_\phi}{2\tau}t]\mathcal{F}_0'(\psi^*(t))\exp[\frac{C_\phi}{2\tau}t] \\
&= \exp[\frac{C_\phi}{\tau}t]\mathcal{F}_0'(\psi^*(t))
\end{aligned}$$

Finally, we have

$$\begin{aligned}
&\frac{\partial}{\partial t}\mathcal{F}(\psi;t) - \left(\frac{1}{2}\frac{C_\phi}{\tau}\psi - \frac{1}{2}\frac{C_\phi}{\tau}\frac{b_0}{a_0}\right)\frac{\partial}{\partial\psi}\mathcal{F}(\psi;t) - \frac{1}{2}\frac{C_\phi}{\tau}\mathcal{F}(\psi;t) \\
= \;& \mathcal{F}_0(\psi^*(t))\frac{C_\phi}{2\tau}\exp[\frac{C_\phi}{2\tau}t] + \psi\mathcal{F}_0'(\psi^*(t))\frac{C_\phi}{2\tau}\exp[\frac{C_\phi}{\tau}t] \\
& -\frac{b_0}{a_0}\frac{C_\phi}{2\tau}\mathcal{F}_0'(\psi^*(t))\exp[\frac{C_\phi}{\tau}t] \\
& -\psi\frac{C_\phi}{2\tau}\exp[\frac{C_\phi}{\tau}t]\mathcal{F}_0'(\psi^*(t)) \\
& +\frac{b_0}{a_0}\frac{C_\phi}{2\tau}\exp[\frac{C_\phi}{\tau}t]\mathcal{F}_0'(\psi^*(t)) \\
& -\frac{C_\phi}{2\tau}\exp[-\frac{C_\phi}{2\tau}t]\mathcal{F}_0(\psi^*(t)) \\
= \;& 0
\end{aligned}$$

This completes the proof.

To find this solution the Favre average has been substituted by the expressions $a(t), b(t)$. In fact these expressions represent the zeroth and first moment of the random variable ϕ. Here, the zeroth and first moment are constant in time. Since we only look at the mixing this result was to expect because it is a requirement for a mixing model as proposed in [17]. We shall see in the next section that the moments are not constant in time if there is also a chemical reaction taking place, i.e. the chemical source term is not zero.

The analytic solution provides a representation of the MDF for a certain initial condition at an arbitrary time t. For a better understanding and to provide insight into the mixing process we discuss a simple example. Typically for mixing problems we start with two different states of the composition variable. This is represented by two δ-distributions at points $\psi^{(1)}$ and $\psi^{(2)}$ in the composition space. Here, we approximate the two delta distributions with Gauß functions because the initial function has to be smooth. These two functions are centered at $\psi^{(1)}$ and $\psi^{(2)}$ and set to zero at some distance from these center to guarantee compact support. Therefore, we can write the initial condition as

$$\mathcal{F}_0(\psi) = \frac{\langle\rho\rangle}{2}\frac{1}{\sqrt{2\pi\sigma^2}}\left(\exp\left(-\frac{(\psi-\psi^{(1)})^2}{2\sigma^2}\right) + \exp\left(-\frac{(\psi-\psi^{(2)})^2}{2\sigma^2}\right)\right). \quad (10)$$

The initial condition, given by equation (10), is displayed in figure 1. We set $C_\phi = 2.0$,$\tau = 1s$, and $\langle\rho\rangle = 1$. This initial condition and the choice of parameters will be used throughout the paper. For the initial condition as given in figure 1 the

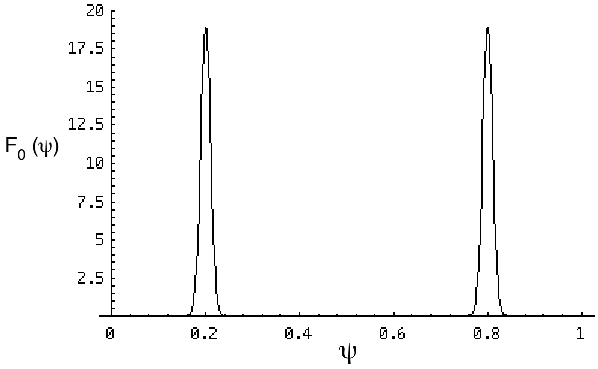

Figure 1: *Two δ-distributions are approximated by Gauß functions with parameters $\sigma = 0.01$ and $\langle\rho\rangle = 1$. The two delta peaks represent two different points in composition space (i.e. $\psi^{(1)} = 0.2$ and $\psi^{(2)} = 0.8$).*

PaSPFR-LMSE models the mixing of two mass streams in a turbulent plug flow reactor. The characteristic curves for this case are shown in figure 2. The mean, as given by the initial distribution at $t = 0$, remains constant in time. In figure 3 the time evolution of the MDF is displayed.

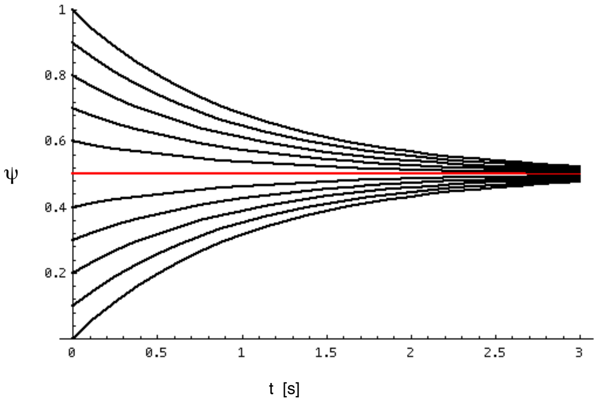

Figure 2: *Characteristic curves for the PaSPFR in the inert case for constant mean mass fraction $\psi = 0.5$ corresponding to the initial condition as given in Figure 1. The mixing time is set to $\tau = 1s$.*

3 PaSPFR-LMSE, First Order Reaction

The PaSPFR-LMSE model equation for the inert case has been solved in the previous section. In this section we consider the simple first order reaction of a species A

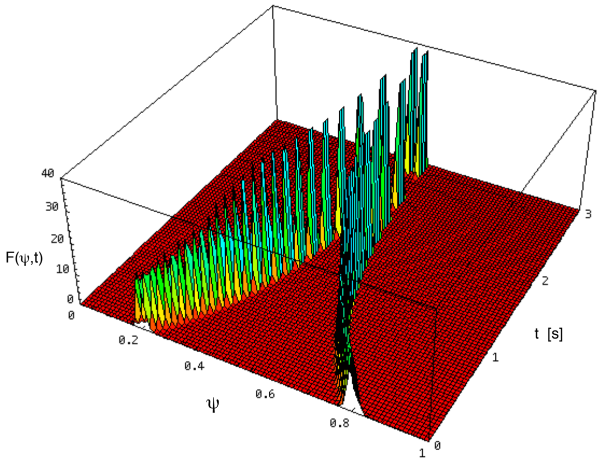

Figure 3: *MDF for inert PaSPFR case. The mass remains constant therefore the maximum values of the MDF increase with time, since the standard deviation of the Gauß functions decrease. The LMSE mixing model (with mixing time $\tau = 1s$) causes the two delta peaks to evolve along the characteristic curves and to tend to a δ at $\psi = 0.5$ with time.*

that reacts to a species B:

$$\mathrm{A} \rightarrow \mathrm{B}. \tag{11}$$

This chemical system with two species A and B can be represented by a one-dimensional hyper plane in the two-dimensional composition space. The mass fraction of the species B can be described by $Y_B = 1 - Y_A$. Therefore it is sufficient to describe the MDF in one dimension only. For this simple isothermal first order reaction (11) the chemical source term is given by $S = -k\psi$. The corresponding transport equation for the MDF, which is also a first order partial differential equation is given as

$$\frac{\partial \mathcal{F}(\psi;t)}{\partial t} = \frac{\partial}{\partial \psi}\Big((\frac{1}{2}\frac{C_\phi}{\tau}(\psi - \tilde{\phi}) + k\psi)\mathcal{F}(\psi;t)\Big) \tag{12}$$

with initial function

$$\mathcal{F}(\psi;0) = \mathcal{F}_0(\psi). \tag{13}$$

For this equation the analytic solution is given in the following Theorem.

Theorem 2 *Let the initial function $\mathcal{F}_0(\psi)$ be sufficiently smooth and assume that at any time $t \in [0,\infty)$ the MDF $\mathcal{F}(\psi;t)$ has compact support in ψ. Then the analytic solution for Cauchy problem (12) and (13) is given by*

$$\mathcal{F}(\psi;t) = \exp((k + \frac{C_\phi}{2\tau})t)\mathcal{F}_0(\psi^*) \tag{14}$$

with

$$\psi^* \; = \; \frac{b_0}{a_0}(1 - \exp(\frac{C_\phi}{2\tau}t)) + \psi \exp(kt + \frac{C_\phi}{2\tau}t), \tag{15}$$

where a_0 is defined as in (8) and b_0 as in (9).

Proof : Proceed as in the previous proof.

In this case mixing and reaction take place simultaneously. Again, as in the inert case, the mixing causes a movement of the two peaks towards the mean. In contrast to the nonreacting case the mean does not remain constant. The calculation of the mean evolution yields the exponential decay of the observed species starting from the mean mass fraction of the initial distribution. The characteristic curves are displayed in figure 4 and the solution, $\mathcal{F}(\psi; t)$, shown in figure 5.

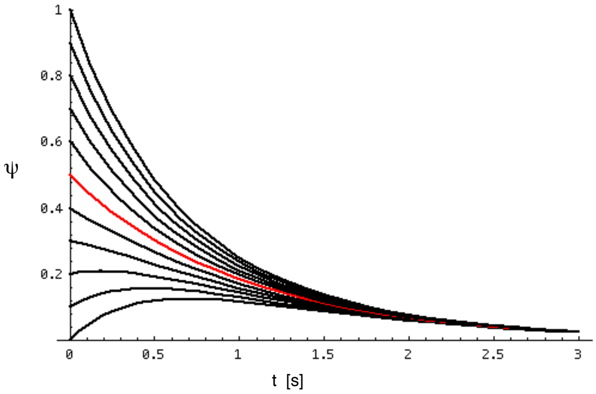

Figure 4: *Characteristic curves for the PaSPFR with LMSE mixing time $\tau = 1s$ and reaction rate constant $k = 1$. At early times mixing causes the characteristic curve, which starts at $\psi = 0.0$ to increase. Simultaneously, the reaction takes place and leads to decreases for larger times.*

4 PaSR, No Mixing, No Reaction

In contrast to the PaSPFR model the PaSR model contains an inhomogeneity that is given by O_4 in equation (1). To understand this term and to have the analytic solution, we first investigate the PaSR equation without mixing and without reactions. This solution has been used in [18, 22] to construct a new particle algorithm for the PaSR equation. This simplified equation is then given by the following partial differential equation.

$$\frac{\partial \mathcal{F}(\psi; t)}{\partial t} \; = \; \frac{1}{\tau_{PaSR}} \left(\mathcal{F}_{in}(\psi) - \mathcal{F}(\psi; t) \right) \tag{16}$$

$$\mathcal{F}(\psi; 0) \; = \; \mathcal{F}_0(\psi) \tag{17}$$

We can now state the following theorem.

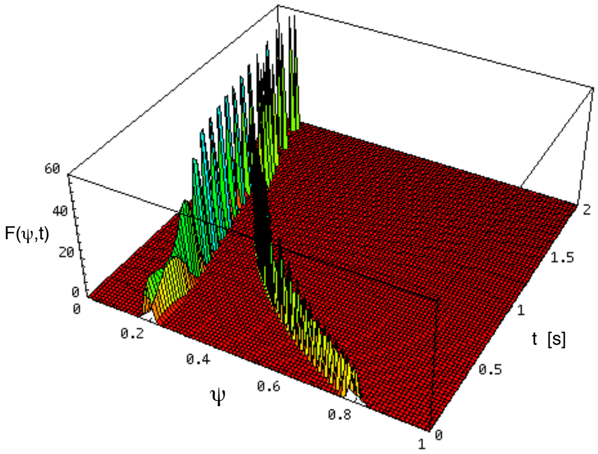

Figure 5: *MDF for the PaSPFR with LMSE mixing model ($\tau = 1s$) and first order chemical reaction (rate constant $k = 1$) for the initial distribution as given in figure 1.*

Theorem 3 *Let the initial data (17) and $\mathcal{F}^{in}$ be sufficiently smooth, then the analytic solution of the Cauchy problem (16), (17) is*

$$\mathcal{F}(\psi;t) = \mathcal{F}_{in}(\psi)(1 - \exp(-\frac{t}{\tau_{PaSR}})) + \mathcal{F}_0(\psi)\exp(-\frac{t}{\tau_{PaSR}}). \tag{18}$$

Proof : Separation of variables.

The solution is displayed in figure 6. In this case the characteristic curves are all constant. The inflow and outflow alters the shape of the MDF.

5 PaSR-LMSE, No Reaction

In this section we consider the more complicated case of PaSR with mixing but no chemical reaction. This means the chemical source term, S, is zero. The first order inhomogeneous partial differential equation and the initial condition is then given by

$$\begin{aligned} \frac{\partial \mathcal{F}(\psi;t)}{\partial t} &- \frac{\partial}{\partial \psi}(\frac{1}{2}\frac{C_\phi}{\tau}(\psi - \tilde{\phi}))\mathcal{F}(\psi;t)) \qquad (19)\\ &= \frac{1}{\tau_{PaSR}}(\mathcal{F}_{in}(\psi) - \mathcal{F}(\psi;t)) \\ \mathcal{F}(\psi;0) &= \mathcal{F}_0(\psi). \qquad (20) \end{aligned}$$

The analytic solution of the PaSR-LMSE for inert mixing is given in the following theorem.

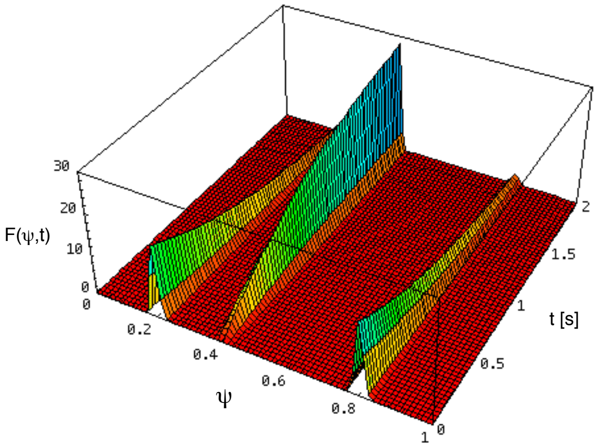

Figure 6: *MDF for the PaSR without mixing and without reaction. The inflow is defined as a Gauß function on the mean mass fraction* $\psi = 0.4$ *with* $\sigma = 0.01$*. The residence time is set on* $\tau_{PaSR} = 3s$*. The initial distribution has been defined as in figure 1*

Theorem 4 *Let the initial data (20) and the inflow* $\mathcal{F}^{in}$ *be sufficiently smooth and assume they have compact support, then the analytic solution of the Cauchy problem (19), (20) is*

$$\begin{aligned}\mathcal{F}(\psi;t) &= \frac{2\tau\mathcal{F}^{in}(\psi^*)}{2\tau - C_\phi\tau_{PaSR}}(1-\exp(t(\frac{C_\phi}{2\tau}-\frac{1}{\tau_{PaSR}}))) \\ &\quad +\exp(t(\frac{C_\phi}{2\tau}-\frac{1}{\tau_{PaSR}}))\mathcal{F}_0(\psi^*)\end{aligned} \tag{21}$$

with

$$\begin{aligned}\psi^* &= \psi\exp(\frac{1}{2}\frac{C_\phi}{\tau}t) \\ &\quad -\frac{1}{2}\frac{C_\phi}{\tau}\int_0^t \frac{b_{in}+b_0\exp(-\frac{t'}{\tau_{PaSR}})-b_{in}\exp(-\frac{t'}{\tau_{PaSR}})}{a_{in}+a_0\exp(-\frac{t'}{\tau_{PaSR}})-a_{in}\exp(-\frac{t'}{\tau_{PaSR}})}\exp(\frac{1}{2}\frac{C_\phi}{\tau}t')dt',\end{aligned} \tag{22}$$

where a_0 *is defined as in (8) and* b_0 *as in (9) and*

$$a_{in} = \int_{-\infty}^{\infty}\mathcal{F}^{in}(\psi)d\psi \tag{23}$$

$$b_{in} = \int_{-\infty}^{\infty}\psi\mathcal{F}^{in}(\psi)d\psi. \tag{24}$$

Proof : Proceed as in the first proof.

To demonstrate the behavior of the solution we choose the residence time $\tau_{PaSR} = 3s$, the mixing time $\tau = 2s$, the initial conditions as in figure 1, and the inflow to be an approximated delta distribution. The characteristic curves are displayed in figure

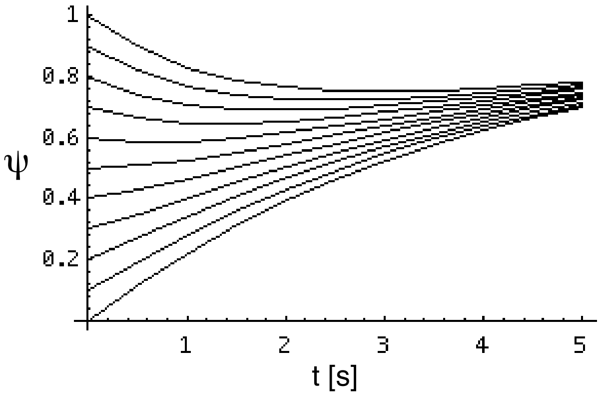

Figure 7: *Characteristic curves for the PaSR with inert mixing at mixing time* $\tau = 2s$ *and residence time* $\tau_{PaSR} = 3s$*. Here the inflow is represented by a Gauß function centered at* $\psi = 0.9$ *with* $\sigma = 0.01$*. In contrast to the last case the characteristic curves tend to* $\psi = 0.9$*.*

7. The residence time determines the speed of change from initial to inflow density. The solution displays the simultaneous processes mixing and inflow, see figure 8. We start with the initial density given in figure 1. The stationary solution corresponds to the inflow condition.

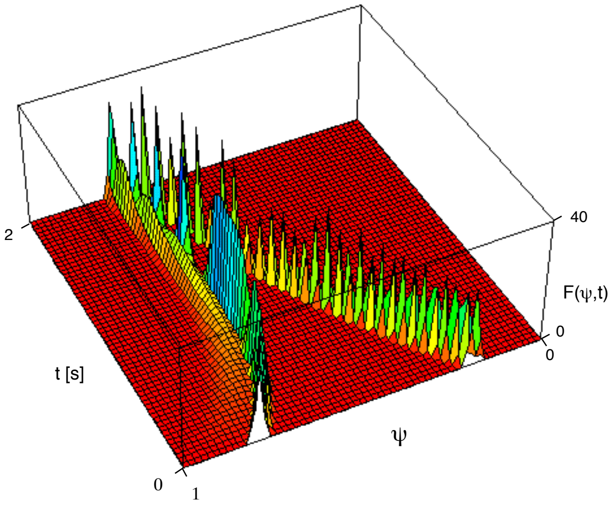

Figure 8: *MDF for the PaSR, inert case with mixing time* $\tau = 2s$ *and residence time* $\tau_{PaSR} = 3s$*.*

6 PaSR-LMSE, First Order Reaction

Finally, we discuss the most complicated case of our examples. The PaSR-LMSE model equation with a first order reaction as given in (11). Hence, the chemical source term is $S = -k\psi$. The inhomogeneous first order partial differential equation with initial data is given by

$$\begin{aligned} \frac{\partial \mathcal{F}(\psi;t)}{\partial t} &- \frac{\partial}{\partial \psi}(\frac{1}{2}\frac{C_\phi}{\tau}(\psi - \tilde{\phi}) + k\psi)\mathcal{F}(\psi;t)) \qquad (25) \\ &= \frac{1}{\tau_{PaSR}}\left(\mathcal{F}_{in}(\psi) - \mathcal{F}(\psi;t)\right) \\ \mathcal{F}(\psi;0) &= \mathcal{F}_0(\psi). \qquad (26) \end{aligned}$$

The solution is given in the theorem.

Theorem 5 *Let the initial data (26) and the inflow* $\mathcal{F}^{in}$ *be sufficiently smooth and assume they have compact support, then the analytic solution of the Cauchy problem (25), (26) is the following*

$$\begin{aligned} \mathcal{F}(\psi;t) &= \frac{2\tau\mathcal{F}^{in}(\psi^*)}{2\tau - C_\phi\tau_{PaSR} - 2k\tau\tau_{PaSR}}(1 - \exp(t(k + \frac{C_\phi}{2\tau} - \frac{1}{\tau_{PaSR}}))) \qquad (27) \\ &\quad + \exp(t(k + \frac{C_\phi}{2\tau} - \frac{1}{\tau_{PaSR}}))\mathcal{F}_0(\psi^*) \end{aligned}$$

with

$$\begin{aligned} \psi^* &= \psi\exp(t(k + \frac{1}{2}\frac{C_\phi}{\tau})) \qquad (28) \\ &- \frac{C_\phi}{\tau}\int_0^t \frac{b_0\exp(t'(-k - \frac{1}{\tau_{PaSR}})) - b_{in}(1 - \exp(t'(-k - \frac{1}{\tau_{PaSR}})))(1 + k\tau_{PaSR})^{-1}}{a_{in} + a_0\exp(-\frac{t'}{\tau_{PaSR}}) - a_{in}\exp(-\frac{t'}{\tau_{PaSR}})} \\ &\quad \times \exp(t'(k + \frac{1}{2}\frac{C_\phi}{\tau}))dt' \end{aligned}$$

where a_0 *is defined as in (8),* b_0 *as in (9),* a_{in} *as in (23), and* b_{in} *as in (24).*

Proof : Proceed as in the proof for the first case.

In figure 9 and 10 the reaction rate constant is chosen as $k = 1$. The reaction has strong influence on the solution. In the steady state inflow and chemical reaction are in a balance determined by the residence time and the reaction rate constant.

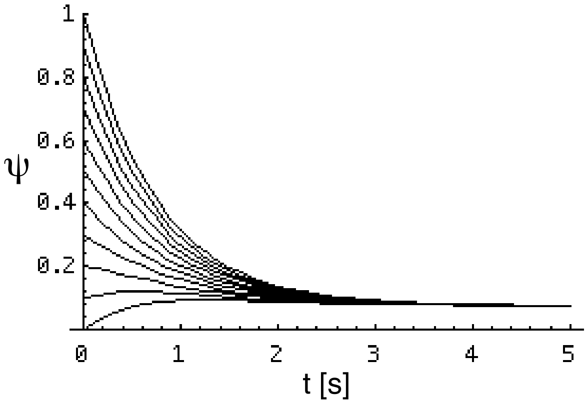

Figure 9: *Characteristic curves for the PaSR with LMSE mixing model at mixing time $\tau = 2s$, reaction rate constant $k = 1$ and residence time $\tau_{PaSR} = 3s$.*

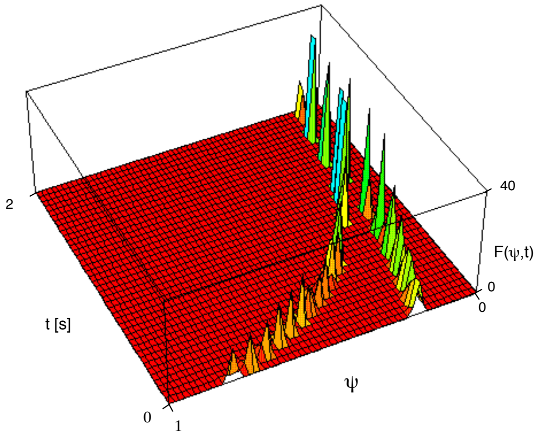

Figure 10: *The solution for the PaSR with LMSE mixing model ($\tau = 2s$), reaction rate constant $k = 1$ and residence time $\tau_{PaSR} = 3s$. The solution starts with two Gauß functions centered at $\psi^{(1)} = 0.2$ and $\psi^{(2)} = 0.8$ with $\sigma = 0.01$ as displayed in figure 1 and an inflow also given as a Gauß function at $\psi^{in} = 0.9$ with $\sigma = 0.01$. The three processes, chemical reaction, mixing and in/outflow interact, and reach a stationary state at $\psi \approx 0.1$.*

7 Conclusion

In this work we presented analytic solutions for the stochastic reactor models PaSPFR and PaSR using the LMSE mixing model. These solutions were obtained by removing the functional dependence of the coefficients in the PaSPFR-LMSE/PaSR-LMSE equation and then applying the method of characteristics to the resulting equation. Five different cases with ascending complexity were discussed. For each case an example was presented that illustrated the typical features of the solution. All cases showed combinations of three different processes: turbulent mixing, chemical reaction, and inflow and outflow. The first case displays the turbulent mixing as given by the LMSE mixing model. In the second case a first order chemical reaction superimposed the mixing process. The third case describes the PaSR model without mixing and without reactions. Cases four and five describe inflow/outflow and mixing effects, without and with first order reaction, respectively. These results can be used for the analysis and construction of numerical schemes for stochastic reactor models but also the full PDF transport equation.

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