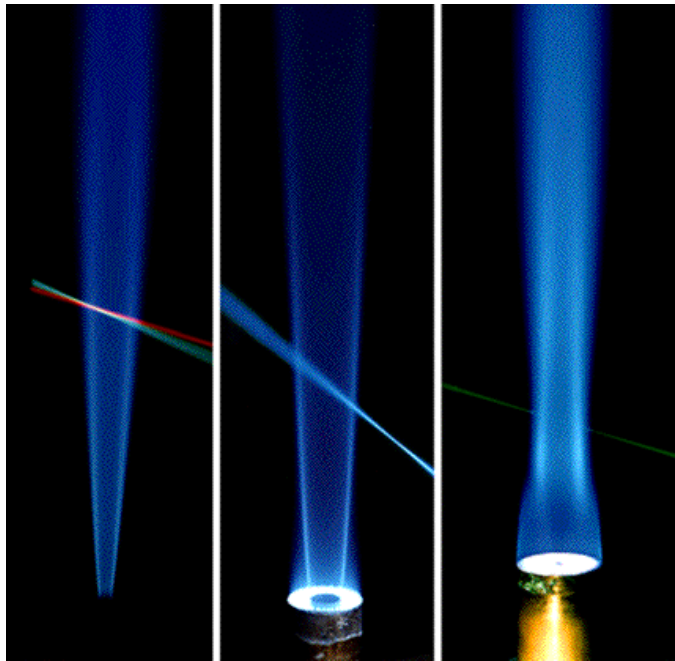




University of Cambridge

Department of Chemical Engineering

Two stochastic approximations of the chemical source term in the PDF transport equation



TNF Workshop

Markus Kraft, Haiyun Su, Sebastian Mosbach

Dept. of Chemical Engineering, University of Cambridge

Wolfgang Wagner

WIAS, Berlin

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Probability Density Function

What describes the PDF ?

Consider the velocity \underline{U} , the scalars $\underline{\psi}$ (chemical species and enthalpy), turbulent frequency ω , and the position \underline{x} to be a random vector. The quantity

$$f(\underline{V}, \underline{\psi}, \theta, \underline{x}, t) dV d\psi d\theta dx$$

describes the probability to find at time t the random vector in the interval

$$\underline{V} \in [\underline{V}, \underline{V} + d\underline{V}]$$

$$\underline{\psi} \in [\underline{\psi}, \underline{\psi} + d\underline{\psi}]$$

$$\underline{x} \in [\underline{x}, \underline{x} + d\underline{x}]$$

$$\theta \in [\theta, \theta + d\theta]$$

Submodels used

- velocity transport
simplified Langevin equation
- scalar transport
IEM interaction by exchange with the mean
- turbulent frequency transport
Van Sloten, Jayesh, Pope



PDF Transport Equation

Mean values are obtained

$$\begin{aligned}\tilde{Q}(\underline{x}) &= \frac{\langle \varrho Q \rangle}{\langle \varrho \rangle} \\ &= \frac{1}{\langle \varrho \rangle} \int_{\underline{V}} \int_{\underline{\psi}} \int_{\theta} Q(\underline{V}, \underline{\psi}, \theta, \underline{x}) \varrho(\underline{\psi}) f(\underline{V}, \underline{\psi}, \theta, \underline{x}) d\underline{V} d\underline{\psi} d\theta\end{aligned}$$

Joint velocity-frequency-composition
PDF Transport Equation

$$\begin{aligned}\frac{\partial \tilde{f}}{\partial t} &= \underbrace{-V_i \frac{\partial \tilde{f}}{\partial x_i}}_{\text{transport in physical space}} \\ &+ \underbrace{\frac{\partial}{\partial V_i} \left(c^U(\underline{V}, \partial_x \langle p \rangle, \langle \varrho \rangle, \tilde{\omega}, \tilde{u}) \tilde{f} \right) + \frac{\partial^2}{\partial V_i^2} \left(d^U(\underline{V}, \tilde{\omega}, \tilde{u}) \tilde{f} \right)}_{\text{transport in velocity space}} \\ &+ \underbrace{\frac{\partial}{\partial \psi_k} \left(M_k(\underline{\psi}, \tilde{\varphi}) \tilde{f} \right) + \frac{\partial}{\partial \psi_k} \left(R_k(\underline{\psi}) \tilde{f} \right)}_{\text{transport in scalar space}} \\ &\quad \underbrace{\text{molecular mixing} \quad \text{chemical reaction}} \\ &+ \underbrace{\frac{\partial}{\partial \theta} \left(c^\omega(\theta, \tilde{\omega}, \tilde{u}_i \tilde{u}_i) \tilde{f} \right) + \frac{\partial^2}{\partial \theta^2} \left(d^\omega(\theta, \tilde{\omega}, \tilde{u}_i \tilde{u}_i) \tilde{f} \right)}_{\text{transport in frequency space}}\end{aligned}$$

$$i = 1, 2, 3 \quad k = 1, \dots, S + 1$$

$$\tilde{f} = \frac{\varrho(\underline{\psi})}{\langle \varrho \rangle} f$$



Numerical Solution

Mass Density Function

$$\mathcal{F}(\underline{U}, \underline{\psi}, \theta, \underline{x}, t) = \varrho(\underline{\psi}) f(\underline{U}, \underline{\psi}, \theta, \underline{x}, t) = \langle \varrho \rangle \tilde{f}(\underline{U}, \underline{\psi}, \theta, \underline{x}, t)$$

Particle System

$$(\Delta m, (\underline{U}^{(n)}(t), \underline{\varphi}^{(n)}(t), \omega^{(n)}(t), \underline{X}^{(n)}(t))^T) \quad n = 1, \dots, N$$

Empirical PDF

$$\mathcal{F}_N(\underline{U}, \underline{\psi}, \theta, \underline{x}) = \Delta m \sum_{n=1}^N \delta(\underline{U}^{(n)} - \underline{U}) \delta(\underline{\varphi}^{(n)} - \underline{\psi}) \delta(\omega^{(n)} - \theta) \delta(\underline{X}^{(n)} - \underline{x})$$

Weak Convergence !

$$\langle \mathcal{F}_N \rangle / \Delta m \sum_{n=1}^N \langle \delta(\underline{X}^{(n)} - \underline{x}) \rangle \xrightarrow{N \rightarrow \infty} \mathcal{F} / \langle \varrho \rangle = \tilde{f}$$

Dynamics of the Particle System

$$d\underline{U}^{(n)} = c^U(\underline{U}^{(n)}, \partial_x \langle p \rangle, \langle \varrho \rangle, \tilde{\omega}, \tilde{u}) dt + \sqrt{d^U(\underline{U}^{(n)}, \tilde{\omega}, \tilde{u})} d\underline{W}$$

$$d\underline{\varphi}^{(n)} = M_k(\underline{\varphi}^{(n)}, \tilde{\varphi}) dt + \underline{R}(\underline{\varphi}^{(n)}) dt$$

$$d\theta^{(n)} = c^\omega(\omega^{(n)}, \tilde{\omega}, \tilde{u}_i \tilde{u}_i) dt + \sqrt{d^\omega(\theta, \tilde{\omega}, \tilde{u}_i \tilde{u}_i)} dW$$

$$d\underline{X}^{(n)} = -\underline{U}^{(n)} dt$$



Numerical Solution

Algorithm

- Initialise Particles
 - uniform distribution in space
 - joint normal distribution for velocities
 - gamma distribution for frequency
- Perform Time Step
 - choose time step according to a CFL condition
 - solve SDE system according to the discretised time step
- Estimate Means
 - particle mesh method (cloud in cell)
 - nonparametric kernel estimation
- Correction Algorithm
 - correct particle positions (continuity)
 - correct velocities (zero divergence, mass flux)
(mean pressure)
 - calculate mean density from particles
- Next Time Step



Challenges

Computational Time

- Administration of Particles
 - advanced data structures and sorting algorithms
- Evaluation of Chemistry
 - QSSA
 - ILDM
 - ISAT (ISAT enhanced)
 - PRISM
 - ANN
- Advantages
 - Faster evaluation of the chemical source term
- Disadvantages
 - Usually a tabulation procedure is required
 - High dimension of the parameter space

Trade off time and storage requirements, and errors

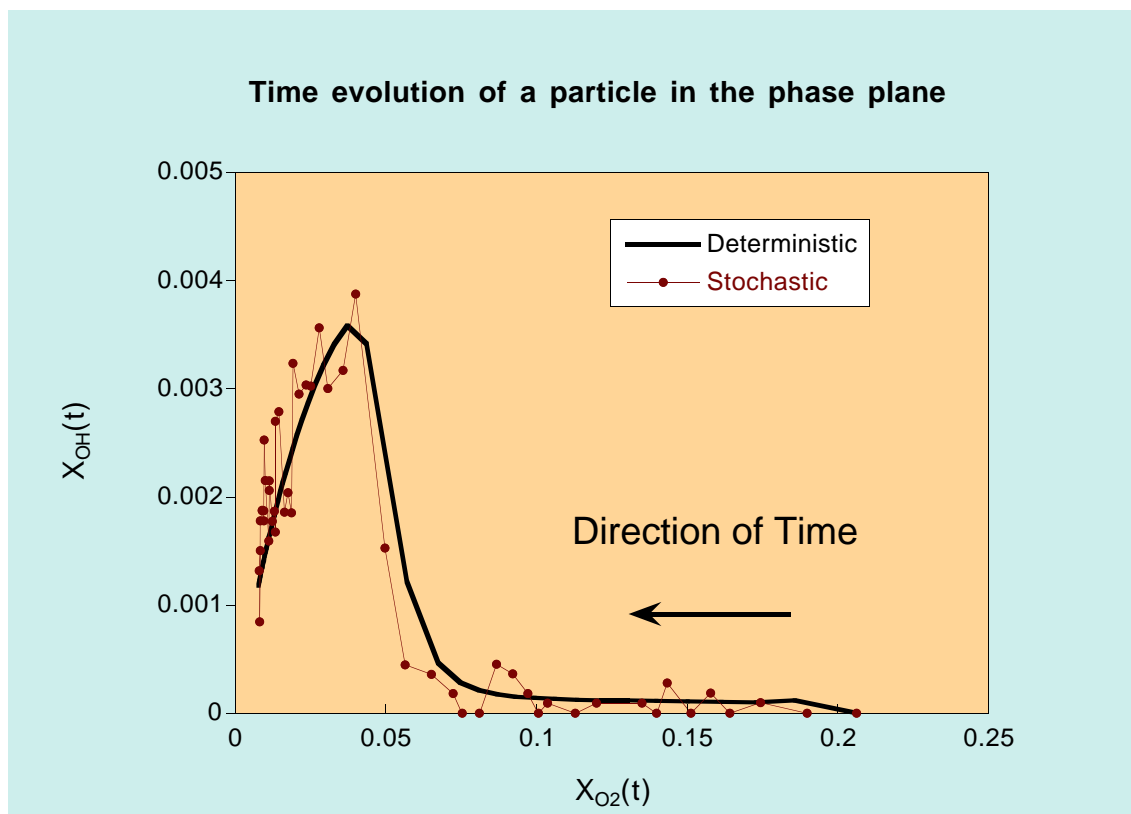


Weak Chemistry

Particles converge only in **weak** sense to the PDF

Dynamics of the scalar component of a particle

$$d\underline{\varphi}^{(n)} = \underbrace{M_k(\underline{\varphi}^{(n)}, \tilde{\varphi})}_{\text{stochastic mixing}} + \underbrace{R(\underline{\varphi}^{(n)})dt}_{\text{deterministic reaction}}$$



We need only **“stochastic trajectories”**!
Can we **construct** a “stochastic trajectory” ?
How **efficient** is this approach?



The PaSPFR Model

The Cauchy Problem

$$\frac{\partial}{\partial t} f(t, \psi) - \sum_{k=1}^{S+1} \frac{\partial}{\partial \psi_k} \left(\left[R_k(\psi) + C M_k(f(t, \psi)) \right] f(t, \psi) \right) = 0,$$

$$f(0, \psi) = f_0(\psi).$$

The components of the vector ψ correspond to the mass fractions Y_1, \dots, Y_S of several chemical species and to temperature T .

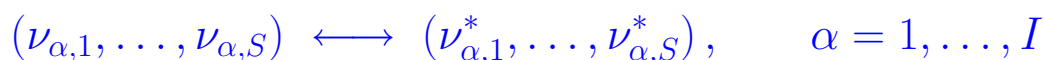
The Mixing Model

We use the IEM mixing model.

$$M_k(g, \psi) = \psi_k - \int \dots \int x_k g(x) dx_1 \dots dx_{S+1}, \quad k = 1, \dots, S+1$$

The Chemistry Model

The terms R_k are given by the **reaction mechanism** of the system, which consists of a number I of elementary chemical reactions,



The stoichiometric coefficients $\nu_{\alpha,i}$ and $\nu_{\alpha,i}^*$ of the species i in reaction α are non-negative integer values.



Particle Method

System of Weighted Particles

$$(w^{(i)}, \Psi^{(i)}(t)) \quad i = 1, \dots, N$$

where

$$\sum_{i=1}^N w^{(i)} = 1$$

Stochastic Trajectories

$$\frac{d}{dt} \Psi_k^{(i)}(t) = -R_k(\Psi^{(i)}(t)) - C \left[\Psi_k^{(i)}(t) - \sum_{j=1}^N w^{(j)} \Psi_k^{(j)}(t) \right]$$

where $k = 1, \dots, S + 1$, and $\Psi^{(i)}(0)$, $i = 1, \dots, N$, are independent and distributed according to f_0 .

Splitting approach

The **high-dimension** requires a splitting approach on a time interval $[s, s + \Delta t]$ to decouple the effects of reaction and mixing.



Particle Method

Reaction step

$$\frac{d}{dt} \tilde{\Psi}_k^{(i)}(t) = -R_k(\tilde{\Psi}^{(i)}(t)), \quad t \geq s, \quad \tilde{\Psi}_k^{(i)}(s) = \Psi_k^{(i)}(s)$$

Mixing step

$$\Psi^{(i)}(s + \Delta t) = e^{-C\Delta t} \tilde{\Psi}^{(i)}(s + \Delta t) + [1 - e^{-C\Delta t}] \sum_{j=1}^N w^{(j)} \tilde{\Psi}^{(j)}(s + \Delta t)$$

Algorithm

0. Determine the state of the system of particles at time 0 according to the initial density f_0 .
1. Given the state of the system at time s , each particle is moved according to the **reaction step**.
2. Given the system $\tilde{\Psi}^{(1)}(s + \Delta t), \dots, \tilde{\Psi}^{(N)}(s + \Delta t)$, each particle is moved according to **mixing step**.
3. If time exceeds termination time then STOP. Otherwise go to Step 1.



The Chemistry Step 1

The Algorithm

Step 0

Fix $n > 0$, set $t = 0$ and initialise the state vector Ψ .

Step 1

Choose a component index k according to the probability

$$P_k = \frac{R_k}{\pi}, \quad \text{where} \quad \pi = \sum_{j=1}^{S+1} R_j$$

is called waiting time parameter.

Step 2

Perform a jump according to

$$\Psi \mapsto J_k(\Psi) = \left(\Psi_1, \dots, \Psi_k - \frac{S}{n} \text{sign} R_k, \dots, \Psi_{S+1} \right),$$

where k is the index chosen in the previous step.

Step 3

Wait an exponentially distributed time τ with waiting time parameter π . That means, advance the time $t \mapsto t + \tau$ such that the waiting time τ is distributed according to

$$\text{Prob}(\tau \geq u) = \exp(-u\pi) \quad \forall u \geq 0.$$

If t exceeds the splitting step Δt then stop, otherwise go to Step 1.



The Chemistry Step 2

A stochastic sub-particle system

$$\Psi = \left(N_1^{(n)}(t), \dots, N_S^{(n)}(t), T^{(n)}(t) \right),$$

The number of sub-particles approximation parameter.

$$n = \sum_{j=1}^S N_j^{(n)}(0)$$

Algorithm

Step 0

The **initial state** of the system is determined as

$$N_j^{(n)}(0) = n X_j(s), \quad j = 1, \dots, S, \quad T^{(n)}(0) = T(s),$$

Step 1

Calculate the **waiting time** τ

$$\text{Prob}(\tau \geq u) = \exp(-u \pi(x)), \quad u \geq 0,$$

where

$$\pi(x) = \sum_{\alpha=1}^I |Q_{\alpha,f}(x) - Q_{\alpha,r}(x)|,$$

and $Q_{\alpha,f}$ and $Q_{\alpha,r}$ are, respectively, the forward and reverse reaction rates. The procedure stops when time $t + \tau$ exceeds the splitting step Δt .



The Chemistry Step 2

Step 2

At the moment $t + \tau$, a particular reaction is chosen according to the **reaction probabilities**

$$P_{\alpha}(x) = \frac{|Q_{\alpha,f}(x) - Q_{\alpha,r}(x)|}{\pi(x)}, \quad \alpha = 1, \dots, I.$$

Step 3

Finally, the process **jumps** into the state

$$J_{\alpha}(x) = \begin{cases} J_{\alpha,f}(x), & \text{if } Q_{\alpha,f}(x) \geq Q_{\alpha,r}(x), \\ J_{\alpha,r}(x), & \text{otherwise,} \end{cases}$$

where

$$J_{\alpha,f}(x) = (x_1 - \nu_{\alpha,1} + \nu_{\alpha,1}^*, \dots, x_S - \nu_{\alpha,S} + \nu_{\alpha,S}^*, x_{S+1} + \Delta T_{\alpha,f}(x))$$

and

$$J_{\alpha,r}(x) = (x_1 - \nu_{\alpha,1}^* + \nu_{\alpha,1}, \dots, x_S - \nu_{\alpha,S}^* + \nu_{\alpha,S}, x_{S+1} + \Delta T_{\alpha,r}(x)).$$

The temperature step is defined as

$$\Delta T_{\alpha,f}(x) = -\frac{\sum_{k=1}^S H_k(x_{S+1}) [\nu_{\alpha,k}^* - \nu_{\alpha,k}]}{\sum_{k=1}^S C_k(x_{S+1}) x_k},$$

$$\Delta T_{\alpha,r}(x) = -\frac{\sum_{k=1}^S H_k(x_{S+1}) [\nu_{\alpha,k} - \nu_{\alpha,k}^*]}{\sum_{k=1}^S C_k(x_{S+1}) x_k}.$$

Then the procedure returns to Step 1.



Approximations

More than 90% of the CPU time is required for updating P_α

Combine two strategies:

- Update C_p, H, V, k_α only if T exceeds a given ΔT
- Update reactions rates not at every reaction event

For a chosen constant ac ,

n_{ac} is the number of reactions with $\pi P_\alpha \geq \frac{ac}{t_{stop}}$.

Table 1: The number of sub-particles and ΔT .

number of sub-particles	$\Delta T(K)$	ac
1.0×10^3	10	-
5.0×10^3	10	-
1.0×10^4	10	-
5.0×10^4	1	2000
1.0×10^5	1	2000

Table 2: n_{ac} and the frequency to update reaction rates.

n_{ac}	The frequency to update reaction rates
greater than 50	50
greater than 25	25
greater than 10	10
others	1



Computational Study

Problem description

non-premixed combustion of n-heptane in hot air

(Detailed mechanism (Westbrook group) 107 chemical species and 808 reversible reactions)

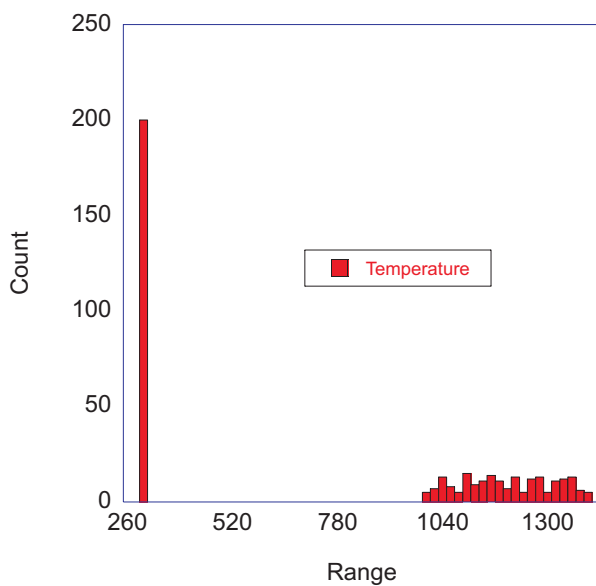
Table 3: Initial concentrations and flow rates.

	Fuel	Air
	\dot{n}_1	\dot{n}_2
	2 mol/min	52 mol/min
$X(\text{nC}_7\text{H}_{16})$	1	0
$X(\text{N}_2)$	0	0.7900
$X(\text{O}_2)$	0	0.2100

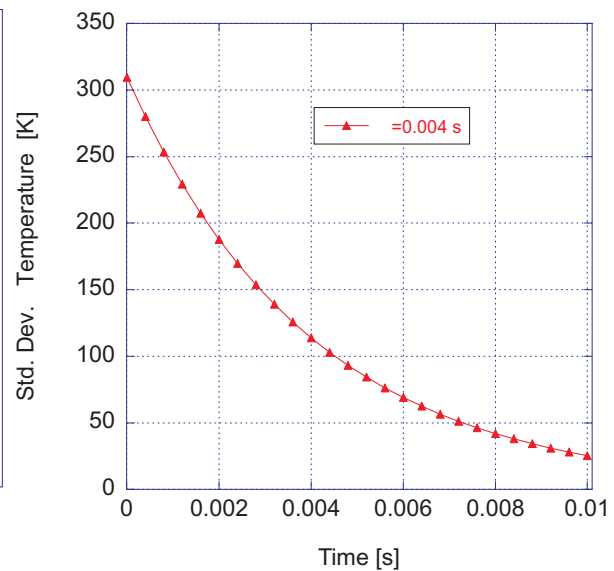
initial condition approximation

Fuel: 50 particles of weight $w^{(i)} = 2.36 \times 10^{-3}$, $i = 1, \dots, 50$,

Air: 50 particles of weight $w^{(i)} = 1.764 \times 10^{-2}$, $i = 51, \dots, 100$,



(a)



(b)



Computational Study

Splitting error

- Difference in mean temperature at the end of the simulation.
- The CPU time grows linearly with the number of splitting steps.
- From the above study we chose the time step $\Delta t = 4.0 \times 10^{-4}$.

Table 4: Splitting error of the temperature at time $t = 0.01$ s.

Δt	error
2.5×10^{-3}	1249.5
1.25×10^{-3}	417.40
6.25×10^{-4}	26.500

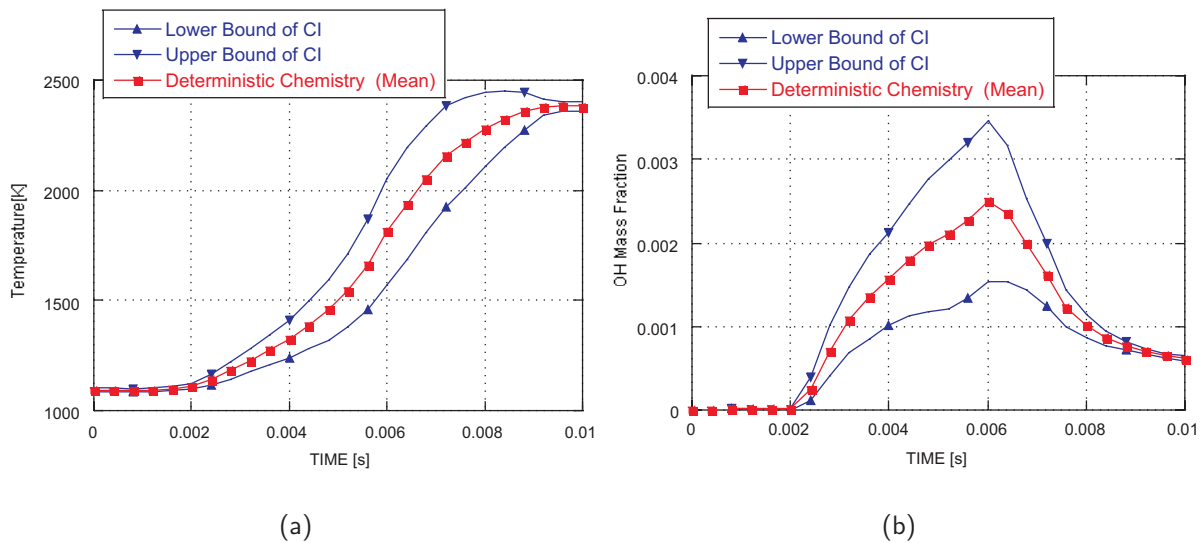


Figure 1: Time evolution of the empirical mean of (a) temperature and (b) OH mass fraction with confidence bounds for 30 repetitions.



Computational Study

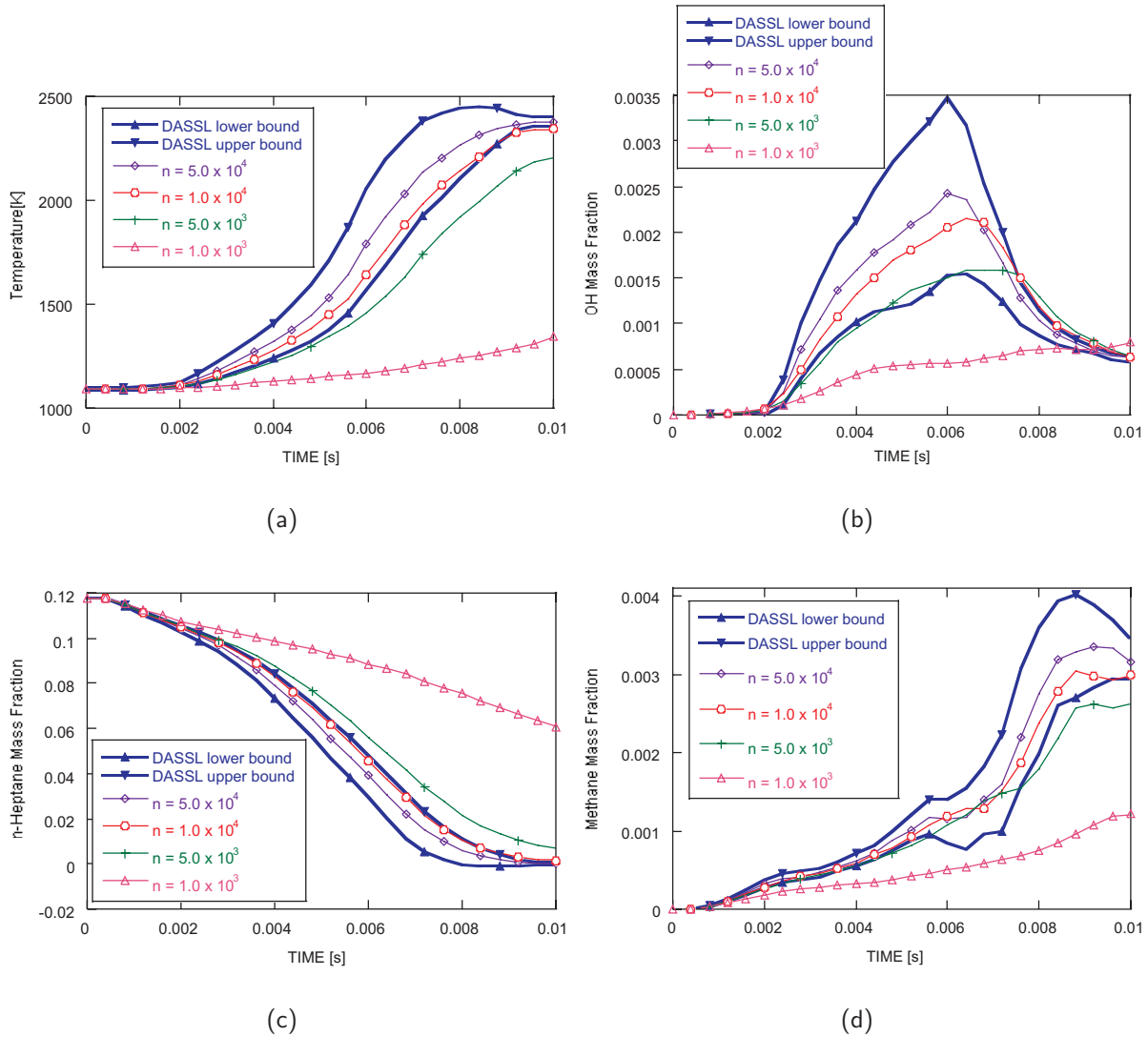


Figure 2: The deterministic chemistry is compared with the stochastic chemistry for three different approximation parameters. The time evolution of the empirical mean of the following quantities is displayed: (a) temperature. (b) OH mass fraction. (c) n-heptane mass fraction. (d) methane mass fraction.



Computational Study

Comparison of stochastic and deterministic chemistry

- The **empirical mean** of temperature, OH mass fraction, n-heptane mass fraction, and methane mass fraction is used for discussion.
- On the basis of the **magnitude of fluctuations** one can consider the result for $n = 1.0 \times 10^4$ to be **sufficiently accurate**. For $n = 5.0 \times 10^3$ the most important characteristics of the ignition are captured.
- **CPU-time** For $n = 10^4$ the algorithm with stochastic chemistry is about **100 times faster** than the algorithm with deterministic chemistry, while it provides a comparable accuracy. In case of $n = 5.0 \times 10^3$ sub-particles, we reach a gain factor of more than 200.

Table 5: Comparison of computational time of deterministic chemistry and stochastic chemistry approximation.

method	CPU time [s]	CPU time of single run [s]	speed factor
DASSL	434,759	14,492	1
5.0×10^4	22,519	751	19.3
1.0×10^4	4,260	142	102
5.0×10^3	2,060	69	211
1.0×10^3	281	9.4	1,547



Summary and Conclusions

Stochastic particle method

- New stochastic chemistry approximation
- **Partial equilibrium modification**
- Incorporation of stochastic chemistry approximation into the PDF transport equation
- **Effect of double averaging**

Numerical Experiments

- **Detailed n-heptane mechanism**
(106 chemical species and 808 reactions)
- Nonpremixed combustion in a PaSPFR
- Study the splitting error
- **Comparison of the stochastic chemistry approach with DASSL**
- Stochastic Chemistry Approximation outperformed DASSL for the cases studied.
- More work needs to be done to achieve more significant speed advantage