System decomposition technique for spray modelling in CFD codes

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Abstract

A new decomposition technique for a system of ordinary differential equations is suggested, based on the geometrical version of the integral manifold method. This is based on comparing the values of the right hand sides of these equations, leading to the separation of the equations into ‘fast’ and ‘slow’ variables. The hierarchy of the decomposition is allowed to vary with time. Equations for fast variables are solved by a stiff ODE system solver with the slow variables taken at the beginning of the time step. The solution of the equations for the slow variables is presented in a simplified form, assuming linearised variation of these variables for the known time evolution of the fast variables. This can be considered as the first order approximation for the fast manifold. This technique is applied to analyse the explosion of a polydisperse spray of diesel fuel. Clear advantages are demonstrated from the point of view of accuracy and CPU efficiency when compared with the conventional approach widely used in CFD codes. The difference between the solution of the full system of equations and the solution of the decomposed system of equations is shown to be negligibly small for practical applications. It is shown that in some cases the system of fast equations is reduced to a single equation.

Keywords: Decomposition, Integral Manifolds Method, Diesel fuel sprays

1 Introduction

Decomposition of complex systems into simpler subsystems is de facto almost universally used in engineering and physics applications. It allows the numerical simulation to focus on the subsystems, thus avoiding substantial difficulties and instabilities related to numerical simulation of the original systems. Special rules are introduced to incorporate the results of numerical simulation of the subsystems into the general scheme of the simulation of the whole system. To the best of our knowledge, the hierarchy of the decomposition process has been so far fixed for the duration of a process.

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As an example of such decomposition we can mention the solutions of ordinary and partial differential equations (ODEs and PDEs) describing spray dynamics in computational fluid dynamics (CFD) codes. Numerical spray modelling is traditionally based on the Lagrangian approach coupled with the Eulerian representation of the gas phase. This permits the decomposition of complicated and highly nonlinear systems of PDEs, describing interactions between computational cells, and the systems of ODEs that govern processes in individual computational cells, including liquid/gas phase exchange and chemical kinetics. The systems of ODEs are usually integrated using much shorter time steps $\delta t$ (typically $10^{-6}$ s) than the global time steps used for calculating the gas phase $\Delta t$ (typically $10^{-4}$ s). Thus the decomposition of ODEs and PDEs is de facto used although its basis has not been rigorously investigated to the best of our knowledge [1, 2].

Further decomposition of the system of ODEs, describing droplets dynamics inside individual computational cells, is widely used. The simplest decomposition of this system of ODEs is based on the sequential solution of individual subsystems comprising this system (split operator approach). In this approach, the solution of each individual subsystem for a given subset of variables is based on the assumption that all the other variables are fixed. The sequence of the solution of individual subsystems is often chosen rather arbitrarily and the results sometimes vary substantially depending on the order in which these subsystems are solved. In the case of a multiscale system, the reliability of this approach becomes questionable altogether, as shown later in Section 4.

We believe that to overcome these problems the multi-scale nature of ODEs needs to be investigated before any attempt to solve them is made. This idea could be prompted by the approaches used in [3] for the analysis of the processes in CO$_2$ lasers and the one used in [4] for the analysis of equations describing the autoignition of diesel fuel (the Shell model). Before solving a system of five stiff ODEs describing five temperatures in these lasers, the characteristic time-scales of these equations were analysed [3]. It was shown that two of these equations describe rather rapid relaxation of two temperatures to the third one. This allowed the authors of [3] to replace the solution of 5 stiff equations by the system of just 3 non-stiff equations without any significant loss of accuracy. The approach used in [4] was different from the one used in [3], but the ultimate result of reduction of the number of ODEs to be solved, and elimination of the stiffness of the system of equations, remained the same. In mathematical terms in both papers the dimension of the ODE system was reduced. In other words, the system was decomposed into lower dimension subsystems.

A similar system decomposition into lower dimension subsystems have been used in constructing reduced chemical mechanisms based on Intrinsic Low-Dimensional Manifolds (ILDM) (e.g. [5] - [7]) and Computational Singular Perturbation (CSP) (e.g. [8] - [12]). There are many similarities between these methods. They are based on a rigorous scale separation such that ‘fast’ and ‘slow’ subspaces of the chemical source term are defined and mechanisms of much reduced stiffness are constructed. These approaches, however, were developed with a view of application to modelling chemical kinetics. Their generalisation to general CFD codes has not been considered to the best of our knowledge.

A useful analytical tool for the analysis of stiff systems of ODEs, used for modelling of spray heating, evaporation and ignition, could be based on the geometrical asymptotic approach to singularly perturbed systems (integral manifold method) as developed by Gol’dshtein and Sobolev [13, 14] for combustion applications (see also [15]). This approach overcomes some of the earlier mentioned problems and is, essentially, focused on systems of ordinary differential
equations of the form:

\[
\frac{dx}{dt} = F(x, y), \quad \varepsilon \frac{dy}{dt} = G(x, y),
\]

where \(x\) and \(y\) are \(n\) and \(m\)-dimensional vector variables, and \(\varepsilon\) is a small positive parameter \((\varepsilon \ll 1)\). The first subsystem \(\frac{dx}{dt} = F(x, y)\) is called a slow subsystem and the second one \(\varepsilon \frac{dy}{dt} = G(x, y)\) is called a fast subsystem. In practical implementations of the integral manifold method a number of simplifying assumptions have been made. These include the assumption that the slow variable is constant during the fast processes. This assumption opened the way to analytical study of the processes \([16] – [19]\).

These approaches to decomposing systems of ODEs were developed and investigated with a view to application to rather special problems, and were based on a number of assumptions. These include fixing of the decomposition over the whole period of the process, and not allowing its hierarchy to change with time. The underlying philosophy of these approaches, however, seems to be attractive for application to the analysis in a wide range of physical and engineering problems including spray modelling in general computational fluid dynamics (CFD) codes. The development of a rather universal new method of decomposition of the system of ODEs, allowing the change of the nature of decomposition with time (dynamic decomposition), will be the main objective of this paper.

As in the original integral manifold method, our formal approach to decomposition of the system of ODEs is based on the division of system variables into ‘fast’ and ‘slow’. This leads to the division of this system onto ‘fast’ and ‘slow’ subsystems. In contrast to the original version of the integral manifold method, however, linearised variations of slow variables during the time evolution of the fast variables will be taken into account as the first order approximation to the fast manifold. The usefulness of this division depends on whether the ‘fast’ subsystem has lower dimension compared with the ‘slow’ subsystem. The procedure can be iterative and result in a hierarchical division of the original system. For example the ‘slow’ subsystem can, in its turn, be subdivided into ‘slow’ and ‘very slow’ subsystems.

The proposed procedure will be initially focused on the simplest possible subdivision of the original system into two subsystems, and applied to spray combustion modelling. Note that ‘fast’ – ‘slow’ decomposition in this case can be different for different phase space regions \([16, 17]\) and for different time intervals. Wider range of application of this method is anticipated.

The preliminary description of this method and its applications was given in \([20]-[22]\).

The general mathematical description of the method and the assumptions on which it is based are presented in Section 2. The rest of the paper discusses application of this method to a specific problem of modelling of sprays. Basic equations describing these processes are presented in Section 3. In Section 4 the results of applying the new method to numerical modelling of these processes are described and discussed. The main results of the paper are summarised in Section 5.

2 Decomposition of the system of equations

Let us consider the system, the state of which is characterized by \(n\) dimensionless parameters, which are denoted as \(Z_n (n = 1, 2, \ldots, n)\). The value of each of these parameters for a given place in space depends on time \(t\), i.e. \(Z_n = Z_n(t)\). This dependence can be found from the
solution of the system of $n$ equations, which can be presented in a vector form:

$$\frac{dZ}{dt} = \Phi(Z), \tag{1}$$

where:

$$Z = (Z_1, Z_2, \ldots, Z_n), \quad \Phi = (\Phi_1, \Phi_2, \ldots, \Phi_n).$$

In the general case, a rigorous coupled numerical solution could be found. This may be not practical, when too many equations are involved. We believe that a more practical approach to this problem could be based on reducing the dimensions of this system as discussed in Introduction. This could be based on organising Equations (1) in terms of decreasing parameter $Y_i$ defined as:

$$Y_i = \frac{\Phi_i(t_k)}{Z_i(t_k)}, \tag{2}$$

where $\Phi_i(t_k) \equiv \Phi_{ik} \equiv \Phi_i(Z_1(t_k), Z_2(t_k), \ldots, Z_i(t_k), \ldots, Z_n(t_k))$ and $Z_i(t_k) \equiv Z_{ik}$ are the right hand sides of Equations (1) and the values of $Z_i$ taken at the time $t_k$ for the time step: $\Delta t : t_k \rightarrow t_{k+1}, \ i = 1, 2, \ldots, n$. For $Z_{ik}$ close to zero we have a special case which requires additional investigation. In practice, in most cases we can just assume that $Z_{ik}$ is a large number.

Note that the Taylor expansion of the right hand side of Equation (1) is:

$$\Phi(Z(t_{k+1})) \equiv \Phi(Z_{k+1}) = \Phi(Z_k) + D\Phi|_{Z=Z_k} (Z_{k+1} - Z_k) + o(Z_{k+1} - Z_k), \tag{3}$$

where $D\Phi$ is the Jacobian matrix of the vector field $\Phi$.

In the general case the value of $\Phi(Z_{k+1})$ is controlled mainly by $\Phi(Z_k)$. However, in the special case where $\Phi(Z_k) = 0$, the second term on the right hand side of Equation (3) becomes dominant. Only in this or similar cases, under certain conditions, Equation (1) can be simplified to:

$$\frac{dZ_i(t_k)}{dt} = \lambda_i(t_k)Z_i(t_k), \tag{4}$$

and the values of $Y_i$ coincide with $\lambda_i$. Our analysis, however, will be focused not on this special case, but on the general case when $Y_i$ is not directly related to $\lambda_i$.

If $Y_i$ is greater than a certain $a\ priori$ chosen positive number $\alpha < 1$, then the corresponding equation can be considered fast and this should be solved rigorously. If the number of ‘fast’ equations is $f \neq 0$, then the system is called multi-scale and this procedure effectively reduces the dimension of the system of Equations (1) from $n$ to $f$. This dimension reduction is particularly attractive when $f$ is small (1 or 2).

In an alternative approach, which turned out to be more practical, we reorganize $Y_i$ in descending order as:

$$Y_{i_1} \geq Y_{i_2} \geq \ldots \geq Y_{i_j} \geq \ldots \geq Y_{i_n}. \tag{5}$$

If we are able to find $j = f$ such that

$$\frac{Y_{i_{j+1}}}{Y_{i_f}} < \epsilon, \tag{6}$$

where $\epsilon$ is another $a\ priori$ chosen small parameter, then we can conclude that the system can be decomposed locally ($\Delta t : t_k \rightarrow t_{k+1}$) into two subsystems: ‘fast’ and ‘slow’. Note that the subscript of $i_j$ just indicates the order in which the parameters are organized (no summation over $f$ in the right hand side of (6) takes place).
Equations for these subsystems can be presented in vector form as:

\[
\frac{d\mathbf{U}}{dt} = \Phi_f \begin{pmatrix} \mathbf{U} \\ \mathbf{V} \end{pmatrix},
\]

(7)

\[
\frac{d\mathbf{V}}{dt} = \Phi_s \begin{pmatrix} \mathbf{U} \\ \mathbf{V} \end{pmatrix},
\]

(8)

where:

\[
\Phi_f = (\Phi_{i_1}, \ldots, \Phi_{i_f}), \quad \Phi_s = (\Phi_{i_{f+1}}, \ldots, \Phi_{i_n}), \quad \mathbf{U} = (Z_{i_1}, \ldots, Z_{i_f}), \quad \mathbf{V} = (Z_{i_{f+1}}, \ldots, Z_{i_n}).
\]

The transformation from the original order of variables

\[
\mathbf{Z} = (Z_1, Z_2, \ldots, Z_n)
\]

to the new order of the same variables

\[
\mathbf{Z}' = (Z_{i_1}, \ldots, Z_{i_f}, Z_{i_{f+1}}, \ldots, Z_{i_n})
\]

was performed with the help of the transformation matrix \( \mathbf{Q} = Q_{i,i_j} \), where \( Q_{i,i_j} = 1 \) when \( i \) corresponds to the original position of the variable, \( i_j \) is the final position of the variable, and \( Q_{i,i_j} = 0 \) for all other \( i \) and \( i_j \). In this case we can formally write:

\[
\mathbf{Z} = \mathbf{Q}(\mathbf{Z}_0) \mathbf{Z}' = \mathbf{Q}(\mathbf{Z}_0) \begin{pmatrix} \mathbf{U} \\ \mathbf{V} \end{pmatrix} = (\mathbf{Q}_f(\mathbf{Z}_0) \quad \mathbf{Q}_s(\mathbf{Z}_0)) \begin{pmatrix} \mathbf{U} \\ \mathbf{V} \end{pmatrix},
\]

(9)

where \( \mathbf{Q} \) is calculated for the values of \( \mathbf{Z} \) at the initial time \( t_0 \) or the beginning of the time step \( (\mathbf{Z}_0) \). The first \( f \) columns of the matrix \( \mathbf{Q} \) refer to the fast subsystem, while the remaining \( n - f \) columns refer to the slow subsystem. This is indicated by introducing the additional matrices \( \mathbf{Q}_f \) and \( \mathbf{Q}_s \).

Note that so far we considered the simplest form of matrices \( \mathbf{Q} \) and \( \mathbf{Q}^{-1} \) performing the change of the order of variables. More complex forms of these matrices could potentially perform the decomposition of the originally non-multiscale system into the multiscale one. Analysis of the latter decomposition, however, is beyond the scope of this paper.

Having introduced a new small positive parameter \( \varepsilon \ll 1 \) and remembering the definitions of \( \mathbf{Q}_f \) and \( \mathbf{Q}_s \) we can rewrite the system of Equations (7) and (8) in a form similar to the one used in Integral Manifold Method:

\[
\varepsilon \frac{d\mathbf{U}}{dt} = \varepsilon \mathbf{Q}_f^{-1}(\mathbf{Z}_0) \Phi \left( \mathbf{Q}(\mathbf{Z}_0) \begin{pmatrix} \mathbf{U} \\ \mathbf{V} \end{pmatrix} \right) \equiv \Phi_{f\varepsilon} \begin{pmatrix} \mathbf{U} \\ \mathbf{V} \end{pmatrix},
\]

(10)

\[
\frac{d\mathbf{V}}{dt} = \mathbf{Q}_s^{-1}(\mathbf{Z}_0) \Phi \left( \mathbf{Q}(\mathbf{Z}_0) \begin{pmatrix} \mathbf{U} \\ \mathbf{V} \end{pmatrix} \right) \equiv \Phi_s \begin{pmatrix} \mathbf{U} \\ \mathbf{V} \end{pmatrix},
\]

(11)

where \( \Phi_{f\varepsilon} = \varepsilon \Phi_f \). In this presentation the right hand sides of Equations (10) and (11) are expected to be of the same order of magnitude over the specified period (time step).

Equations (10) and (11) will be integrated over the time period \( \Delta t : t_k \rightarrow t_{k+1} \). The zeroth order solution of Equation (11) is just a constant value of the slow variable: \( \mathbf{V}_k^0 = \mathbf{V}_k = ((Z_{i_{f+1}k}, \ldots, Z_{in}k), \) where the superscript \(^0\) indicates the zeroth approximation, while the
subscripts \( k \) and \( k+1 \) indicate the point in time. The zeroth order for the fast variable is found from Equation (10) with \( \mathbf{V} = \mathbf{V}_k \). This could be interpreted as the equation for the slow variable on the fast manifold. This means that Equation (10) (or (7)) is approximated by the following system:

\[
\frac{d\mathbf{U}}{dt} = \Phi_f \begin{pmatrix} \mathbf{U} \\ \mathbf{V}_k \end{pmatrix}.
\]  

(12)

The solution of Equation (12) at \( t = t_{k+1} \) (\( \mathbf{U}^{(0)}_{k+1} \)) is the zeroth order approximation of the fast motion on the fast manifold at \( t = t_k \). Note that the system of Equations (12) can be stiff in the general case, but with a reduced level of stiffness, compared with the original system (1). Hence, the suggested method is expected to reduce the level of stiffness of the system and not to eliminate the stiffness altogether.

Under the same zeroth order approximation the slow variables would remain constant over the same time step. This assumption was used in the original formulation of the Method of Integral Manifolds [14]. This, however, might lead to an unphysical result when slow variables would remain constant for any time \( t > t_0 \). Hence, the need to calculate slow variables using at least the first order approximation. In the case when \( \varepsilon \) is not asymptotically small, further, or higher order, approximations need to be considered. In this case we introduce the new time scale \( \tau = 1/\varepsilon \), and formally present the slow and fast variables as:

\[
\begin{align*}
V(\tau) &= V^{(0)} + \varepsilon V^{(1)}(\tau) + \varepsilon^2 V^{(2)}(\tau) + \ldots, \\
U(\tau) &= U^{(0)}(\tau) + \varepsilon U^{(1)}(\tau) + \varepsilon^2 U^{(2)}(\tau) + \ldots
\end{align*}
\]

(13)

Having substituted Expressions (13) into Equation (11) we obtain:

\[
\frac{d(V^{(0)} + \varepsilon V^{(1)}(\tau) + \varepsilon^2 V^{(2)}(\tau) + \ldots)}{d\tau} = \varepsilon \Phi_s \begin{pmatrix} U^{(0)}(\tau) + \varepsilon U^{(1)}(\tau) + \varepsilon^2 U^{(2)}(\tau) + \ldots \\ V^{(0)} + \varepsilon V^{(1)}(\tau) + \varepsilon^2 V^{(2)}(\tau) + \ldots \end{pmatrix}.
\]

(14)

Equation (14) allows us to obtain the first order solution for the slow variable in the form:

\[
V_{k+1} = V_k^{(0)} + \varepsilon V_{k+1}^{(1)} = V_k^{(0)} + \varepsilon \Phi_s \begin{pmatrix} U_{k+1}^{(0)} \\ V_k^{(0)} \end{pmatrix} \Delta \tau.
\]

(15)

Returning to the original variables we can write the expression for the value of \( \mathbf{V}(t_{k+1}) \equiv \mathbf{V}_{k+1} \) in the form:

\[
\begin{align*}
\mathbf{V}_{k+1} &= \mathbf{V}_k^{(0)} + \Phi_s \begin{pmatrix} U_{k+1}^{(0)} \\ V_k^{(0)} \end{pmatrix} \Delta t \\
&= \left( Z_{i+1, k} + \Phi_{i+1} \begin{pmatrix} U_{k+1}^{(0)}, V_k^{(0)} \end{pmatrix} \Delta t, \ldots, Z_{i, k} + \Phi_i \begin{pmatrix} U_{k+1}^{(0)}, V_k^{(0)} \end{pmatrix} \Delta t \right).
\end{align*}
\]

(16)

To increase accuracy of calculations one could continue the process to take into account the first order solution for the fast motion. Then the second order solution for the slow motion could be obtained etc..

Since the above mentioned decomposition of the original system of equations is allowed to vary with time, we suggest to call this dynamic decomposition approach.
3 Basic equations for spray modelling

In this section basic equations used for modelling droplets heating, evaporation and combustion will be summarised. These equations will be presented in the general form, following [23, 24], and in the simplified form (partly following [25]). The latter form of these equations will allow us to perform a direct comparison between the predictions of conventional CFD approach, and the approach described in this paper. A number of processes, including droplet dynamics, break-up and coalescence, and the effects of temperature gradient inside droplets will be ignored at this stage (see [26]-[32]). This can be justified by the fact that the main emphasis of this paper will be on the investigation of the new method of the solution of the systems of ODEs relevant to spray combustion modelling rather than providing a detailed analysis of the processes involved.

**Droplet mass**

As shown in [23, 32], the equation for stationary droplet mass $m_d$ can be presented as:

\[
\dot{m}_d = 4\pi \bar{k}_g R_d c_{pF} \ln(1 + B_T),
\]

(17)

where

\[
B_T = \frac{c_{pF}(T_g - T_s)}{L_{eff}}
\]

is the temperature Spalding number,

\[
L_{eff} = L(T_s) + \frac{Q_L}{\dot{m}_d}
\]

$L$ is the specific latent heat of vaporization, $Q_L$ is the heat spent on droplet heating, $\bar{k}_g$ is the average gas thermal conductivity, $R_d$ is droplet radius, $c_{pF}$ is specific heat capacity of fuel vapour.

Analysis of Equation (17) is not trivial and requires iterations [23]. To test the new system dimension reduction technique we will use a much simpler form of this equation [25]:

\[
\dot{m}_d = 4\pi \bar{k}_g R_d c_{pF} \ln(1 + B_M),
\]

(18)

where $B_M = (Y_{fs} - Y_{f\infty})/(1 - Y_{fs})$ is the Spalding mass number, $Y_{fs}$ and $Y_{f\infty}$ are the mass fractions of fuel vapour near the droplet surface and in the ambient gas respectively. We present the expression for $Y_{fs}$ as:

\[
Y_{fs} = \left[ 1 + \left( \frac{p}{p_{fs}} - 1 \right) \frac{M_a}{M_f} \right]^{-1},
\]

(19)

$p$ and $p_{fs}$ are ambient pressure and the pressure of saturated fuel vapour near the surface of droplets respectively, $M_a$ and $M_f$ are molar masses of air and fuel; $p_{fs}$ can be calculated from the Clausius-Clapeyron equation presented in the form [25]:

\[
p_{fs} = \exp \left[ a_f \frac{b_f}{T_s - 43} \right],
\]

(20)
\(a_f\) and \(b_f\) are constants to be specified for specific fuels, \(T_s\) is the surface temperature of fuel droplets in K; \(p_{fs}\) predicted by Equation (20) is in kPa. We assumed that \(Le=1\), and ignore the temperature dependence of liquid density, gas thermal conductivity and viscosity. In the calculations we took the values \(a_f = 15.5274\) and \(b_f = 5383.59\) recommended for diesel fuel [25].

**Droplet temperature**

Following [23, 33, 34] we can present the equation for stationary droplet temperature as:

\[
m_d c_l \frac{dT_d}{dt} = 4\pi R_d^2 h(T_g - T_d) - \dot{m}_d L + 4\pi R_d^2 \sigma \overline{Q}_a \theta_R^4,
\]

where

\[
Nu = \frac{2hR_d}{k_g} = 2 \ln(1 + B_T) \frac{1}{B_T},
\]

\(\theta_R\) is the radiative temperature, as calculated from P-1 model (as the starting point we assume that \(\theta_R = T_{ext}\) (external temperature)), \(\overline{Q}_a\) is the average absorption efficiency factor, which can be calculated from the equation:

\[
\overline{Q}_a = a_r R_d^b,
\]

\(a_r\) and \(b_r\) are polynomials of \(\theta_R\), \(c_l\) is liquid specific heat capacity.

To test the new system dimension reduction technique the effect of thermal radiation will be ignored and we use a simplified form of the temperature dependence of \(L\) [25]:

\[
L = L_{T_{bn}} \left( \frac{T_{cr} - T_s}{T_{cr} - T_{bn}} \right)
\]

where \(L_{T_{bn}}\) is the value of \(L\) at the droplet boiling temperature \(T_{bn}\), \(T_{cr}\) is the critical temperature. Following [25] we assume that \(T_{bn} = 536.4\) K, \(T_{cr} = 725.9\) K, and \(L_{T_{bn}} = 254000\) J/kg. Also, we assume that \(B_T = B_M\) and liquid density is constant.

Equations (18) and (21), written for individual droplets, will be applied to describe droplet parcels, following the conventional approach widely used in computational fluid dynamics codes.

**Fuel vapour density**

This equation follows directly from the conservation of fuel vapour:

\[
\alpha_g \frac{d\rho_{fv}}{dt} = -\alpha_g CT + \left[ \sum_i \dot{m}_{di} / V \right],
\]

where \(\rho_{fv}\) is the fuel vapour density, \(\alpha_g\) is the volume fraction of gas assumed equal to 1 in our calculations, the summation is assumed over all droplets in volume \(V\), \(Q_f\) is the heat released per unit mass of burnt fuel vapour (in J/kg), \(CT\) is the chemical term describing fuel depletion (in kg/(m³s)).

Following [35] we use the expression of the rate of reaction in the form:

\[
k_{cr} = A[\text{fuel}]^a[O_2]^b \exp\left[-E/(BT)\right],
\]
where \( k_c \) has units of mole/(cm\(^3\)·s), while the concentrations of fuel [fuel] and oxygen \([O_2]\) has units of mole/cm\(^3\). The values of these coefficients given for C\(_{10}\)H\(_{22}\) will be used. These are the closest to n-dodecane (C\(_{12}\)H\(_{26}\)) (the closest approximation for diesel fuel) [35]:

\[
A = 3.8 \times 10^{11} \left( \frac{\text{mole}}{\text{cm}^3} \right)^{1-a-b} = 2.137 \times 10^9 \left( \frac{\text{k mole}}{\text{m}^3} \right)^{1-a-b};
\]

\[
E = 30 \frac{\text{kcal}}{\text{mole}} = 1.255 \times 10^8 \frac{\text{J}}{\text{kmole}}; \quad a = 0.25; \quad b = 1.5.
\]

Using \( A \) in \( \left( \frac{\text{mole}}{\text{cm}^3} \right)^{1-a-b} \) and \( E \) in \( \frac{\text{J}}{\text{kmole}} \), we can write:

\[
CT = A \ M_{O_2}^{1.5} \ M_f^{0.75} \rho_f^{0.25} \ O_2^{1.5} \exp \left( -\frac{E}{(BT)} \right), \tag{26}
\]

where \( M_{O_2} = 32 \ \text{kg/kmol} \), and \( M_f = 170 \ \text{kg/kmol} \) are molar masses of oxygen and fuel respectively in kg/kmole, \( \rho_{O_2} \) is the density of oxygen.

In the case of diesel engines, one of the most widely used autoignition chemical models is the so called Shell model [1, 4, 36].

**Density of Oxygen**

A single step global reaction for n-dodecane combustion can be written as:

\[
C_{12}H_{26} + 18.5O_2 \rightarrow 12CO_2 + 13H_2O.
\]

Hence the equation for density of Oxygen can be presented as:

\[
\frac{d\rho_{O_2}}{dt} = -18.5 \ \frac{M_{O_2}}{M_f} CT = -3.48235 \ \text{CT}. \tag{27}
\]

A useful characteristic, widely used as a measure of reactivity of the fuel vapour /air mixture is the equivalence ratio:

\[
\varphi = \frac{\text{Fuel}/\text{Air}}{(\text{Fuel}/\text{Air})_{\text{stoich}}} = \frac{\text{Fuel}/\text{Oxygen}}{(\text{Fuel}/\text{Oxygen})_{\text{stoich}}} = 18.5 \times \frac{\rho_f}{\rho_{O_2}} = \frac{3.48\rho_f}{\rho_{O_2}},
\]

where \((\text{Fuel}/\text{Air})_{\text{stoich}}\) is the stoichiometric ratio of the densities of fuel and air.

**Gas temperature**

The condition of energy balance leads us to the following equation for gas temperature:

\[
c_{\text{mix}}\rho_{\text{mix}} \frac{dT_g}{dt} = \alpha_g Q_f CT - \left[ \sum_i m_{di} c_l \frac{dT_{di}}{dt} + \sum_i \dot{m}_{di} L + \sum_i \dot{m}_{di} c_p(T_g - T_{di}) \right] / V. \tag{28}
\]
4 Application

The method described in Section 2 will be applied to simulate polydisperse spray heating, evaporation and ignition. The model on which the analysis is based is chosen to be rather simple, but capable nevertheless of capturing the essential features of the process. We consider 3 droplets with initial radii 5 μm, 9 μm and 13 μm respectively. The initial temperatures of all droplets is taken to be equal to 400 K. The gas temperature is taken to be equal to 880 K [1]. The gas volume is chosen such that if the droplets are fully evaporated without combustion then the equivalence ratio of fuel vapour/air mixture is equal to 4. This is the situation typical for diesel engines in the vicinity of the nozzle. The initial density of Oxygen is taken to be equal to 2.73 kg/m³ (this corresponds to air pressure equal to 3 MPa). The initial mass fraction of fuel is taken to be equal to zero. These values of the parameters can be considered as an approximation of the actual conditions in diesel engines [1].

The calculations were based on Equations (18), (21), (24) – (27) and the equation for the density of the mixture \( \rho_{\text{mix}} \) of fuel vapour and air:

\[
\frac{d\rho_{\text{mix}}}{dt} = \sum_i \frac{d\rho_i}{dt},
\]

(29)

where \( \rho_i \) are the densities of individual components. The calculations were performed until gas temperature reached 1100 K. At this temperature the autoignition process was assumed to be completed [1]. Since Equations (18) and (21) are solved for 3 droplets, the maximal number of equations to be solved was equal to 10. Note that the density of the fuel vapour/air mixture could be derived algebraically from mass conservation. It was prefered, however, to solve the ODE for it to enable us to monitor the mass conservation in the system as a validity check.

Once the smaller droplets have evaporated, the number of equations was reduced. These coupled equations were solved using three approaches.

Firstly, following widely used practice in CFD codes, the system of equations was divided into subsystems which were solved sequentially. This approach is widely referred to as the operator splitting technique (see [37]). These subsystems include equations for mass and temperature of each droplet (three subsystems) and equations for gas temperature, fuel, Oxygen and mixture density (additional fourth subsystem). When each of these subsystems was solved, the remaining variables were assumed to have constant values over the time step. This paper refers to this approach as ‘fixed decomposition approach’ to distinguish it from the ‘dynamic decomposition approach’ discussed in Section 2. More specifically, at the first step equations for the mass and the temperature of each droplet (Equations (18) and (21)) were solved simultaneously (3 systems of equations). Then the results were used to calculate the density of fuel and mixture, and temperature of gas without taking into account the chemical term (see Equations (24) (29) and (28)). Next, the chemical term was calculated based on Equation (26), and the result was used to calculate the density of Oxygen (Equation (27)). Finally, the values of the density of fuel and mixture, and temperature of gas were updated using the chemical term. This approach is effectively equivalent to the simplest form of (A-B) splitting as described in [37].

Secondly, these equations were solved rigorously using DLSODAR stiff solver from ODEPACK developed in LLNL laboratory. This means that all equations were solved simultaneously in a coupled way.
The third approach is based on decomposing of the original system following the procedure described in Section 2 with $\epsilon = 0.25$. Note that this parameter is not related to the parameter $\varepsilon$ used in Equations (10) and (13). The total number of equations solved, and the number of equations for fast variables could change with time as expected. The corresponding plots of the numbers of these equations are shown in Fig. 1. As follows from this figure, initially all 10 equations were solved, when the first or second approaches were used. Then this number was reduced to 8 when the smallest droplet evaporated, and to 6 when two smallest droplets evaporated. Initially, the number of equations for fast variables to be solved was equal to 4, then it dropped to just one equation describing fuel vapour density. Between about 0.25 ms and 0.5 ms the number of equations for fast variables was equal to two (equations for fuel vapour density and the radius of the smallest droplet). Then again just the equation for fuel density was solved. Between about 0.6 ms and 0.8 ms the number of fast equations to be solved is comparable with the total number of equations solved. During this period the decomposition of the system is not expected to be useful. After about 0.8 ms and until about 1.8 ms only one equation (fuel density) or two equations (fuel density and the radius of the second droplet) were used. In this case the decomposition technique described in Section 2 is expected to be particularly important.

The time evolution of gas temperature, equivalence ratio and the radius of the largest droplet, calculated using the abovementioned three approaches, are shown in Figs. 2 – 4 respectively. Fig. 2 appears to be the most informative and practically important, as it indicates the total ignition delay time, i.e. the time required for the gas to reach 1100 K. As follows from Fig. 2, the first approach appears to be very sensitive towards the time step chosen. If the time step $10^{-4}$ s is chosen then the predicted total ignition delay is almost four times longer than the one predicted based on the second approach (coupled solution of the whole system). If the time step is decreased to $5 \times 10^{-5}$ s and $10^{-5}$ s then calculations using the first method appear to be more accurate than in the case when this time step is equal to $10^{-4}$, but still the accuracy of computations is hardly acceptable for practical applications. Even for a rather small time step, $10^{-5}$ s, the predicted total ignition delay is more than 20% greater than predicted by the rigorous coupled solution of this system of equations (second approach).

The application of the third approach to the solution of this system gives a rather different picture. Even in the case of the largest time step ($10^{-4}$ s) the error of calculations of the total ignition time delay was just 13%. In the case of smaller time steps, the time delay predicted by solving the decomposed system almost coincides with the one obtained by rigorously solving the whole system with possible errors not exceeding 2%. Essentially the same conclusion regarding the benefits of the third approach based on the decomposition of the original system of equations follows from Figs. 3 and 4, showing the time evolution of the instantaneous equivalence ratio and the radius of the largest droplets. Also, the difference of the values of other variables, predicted by the solutions of the system, using the above mentioned three approaches, was observed.

At the next step the solution of equations was performed for a different set of parameters, typical for the peripheral region of fuel sprays in diesel engines [1]. We consider 3 droplets with initial radii 5 $\mu$m, 9 $\mu$m and 17 $\mu$m respectively. The gas temperature is taken equal to 780 K [1]. The gas volume is chosen such that if the droplets are fully evaporated without combustion then the equivalence ratio of fuel vapour/air mixture is equal to 1. As in the previous case, the initial density of Oxygen and the initial droplet temperatures are taken equal to 2.73 kg/m$^3$ and 400 K respectively. The initial mass fraction of fuel is taken equal to zero. The plots of
the number of equations solved using the above mentioned three approaches are shown in Fig. 5. Between about 0.1 ms and 0.4 ms only one equation for the temperature of the smallest droplet was solved when the third approach was used. In general, the decomposition technique described in Section 2 is expected to be particularly useful in the ranges 0.1 – 0.7 ms and 1 – 2.4 ms when not more than two equations for fast variables were solved.

The plots of time evolution of gas temperature, calculated using the abovementioned three approaches, are shown in Fig. 6. The calculations were performed for the same $\Delta t$ s as in the case shown in Fig. 2, but the results are shown just for $\Delta t = 10^{-5}$ s. The dependence of the results on $\Delta t$ in the range of values of this parameter under consideration ($\Delta t = 10^{-5} - 10^{-4}$ s) turned out to be weak and the plots almost coincided. The comparison of the three curves in this figure shows that the solution of the decomposed system in this case turned out to be far more accurate than the solution used in CFD codes (first approach).

To compare the CPU efficiency of the new (dynamic decomposition) and conventional CFD (fixed decomposition) approaches, a series of runs for various time steps were performed for both cases considered in this section. A polydisperse spray including three droplet parcels, 10,000 droplets each, was injected at the start of the calculation. For fixed time steps the CPU requirements of both approaches were about the same. As shown above, however, the accuracy of the new approach was always higher than that of the conventional approach. Thus the comparison of CPU requirements of both methods for fixed time steps would be misleading. An alternative approach needs to take into account the accuracy of calculations. As followed from our calculations, the autoignition delays predicted by the dynamic decomposition approach coincided with those predicted by the full coupled solution of the system of equations for the time step of $10^{-6}$ s. This value of the autoignition delay was considered as the true value for further comparisons. For example, for the second set of parameters errors less than 1.5% were achieved for time step of $1.3 \times 10^{-5}$ s for the conventional CFD approach, and for time step of $2.4 \times 10^{-5}$ s for the new approach. When this effect was taken into account then in all cases under consideration, the CPU time for the new method was always smaller than that for the conventional approach. In some cases, the CPU reduction for the new approach was as high as factor of 3. The CPU time was estimated based on the customised function DATE_AND_TIME. The standard function GETTIME did not give consistent results for small CPU times.

A number of additional tests has been conducted to compare the performances of the standard fix decomposition approach (used in CFD codes) and the new dynamic decomposition method. Both programs were run sequentially on two workstations (Silicon Graphics, Intel 64bit processor) and using two Fortran Compilers (Intel – Fortran 95, GNU – Fortran 77) with the additional option of code optimisation. The above mentioned customised function DATE_AND_TIME was used to estimate the CPU time required for system integration. It has been found that, for a given time step and for a low level of code optimisation, the CPU time is less for the standard fix decomposition approach, whereas an increase in the level of optimisation leads to comparable times required for program execution. For example, for the case shown in Figs. 1-4 for the time step $\Delta t = 5 \times 10^{-5}$, the average time of the program execution with the code optimisation level set to O0 (i.e. no code optimisation) was approximately equal to 0.12 s for the fixed decomposition approach and 0.21 s for the dynamic decomposition approach. For the optimisation level set to O2 (this option is the default one, it enables optimisations for speed, including global code scheduling, software pipelining, prediction, speculation etc.) these times become 0.15 s and 0.13 s respectively. Therefore further improvements of real-
isation of the dynamic decomposition method are possible and might be implemented, leading to optimising the realisation structure of the code and numerics.

Note that the coupled solution of the system of equations using the stiff solver is always more accurate than the solutions based on dynamic and fixed decompositions, and is usually more CPU efficient. Hence, in the case when the number of equations is relatively small (as in the cases considered in this section) there is no need to develop any decomposition technique at the first place. However, in realistic engineering calculations, when the number of droplet parcels could be tens of thousands [1], no stiff solver can cope with the full coupled system of ODEs describing them. The real competition in this case is between fixed and dynamic decomposition approaches as described above. In our paper the coupled solution of the full system of equations was used for estimation of the accuracy of these two approaches.

5 Conclusions

A new method of numerical solution of multiscale systems of ordinary differential equations (ODEs) is suggested. This is based on a decomposition technique for systems of ordinary differential equations, using the geometrical version of the Integral Manifold Method. The comparative analysis of the values of the right hand sides of these equations, can result in the separation of the equations for ‘fast’ and ‘slow’ variables. The hierarchy of the decomposition is allowed to vary with time. Hence, this decomposition is called dynamic. Equations for fast variables are solved by a stiff ODE system solver with the slow variables taken at the beginning of the time step. This is considered as a zeroth order solution for these variables. The solution of equations for slow variables is presented in a simplified form, assuming linearised variations of these variables during the time evolution of the fast variables. This is considered as the first order approximation for the solution for these variables or the first approximation for the fast manifold. This approach is applied to the analysis of the problem of explosion of a polydisperse spray of diesel fuel for the parameters typical for the vicinity of the nozzle and the periphery of the spray. Our results show clear advantages of the new approach from the point of view of accuracy and CPU efficiency when compared with the conventional approach widely used in CFD codes. The latter is called the fixed decomposition approach. The difference in the solutions of dynamically decomposed and full systems of equations is shown to be negligibly small for practical applications.

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References


**Figure captions**

**Fig. 1** Plots of the total number of equations solved (dashed) and the number of equations for fast variables (solid) for the values of parameters as specified in the text. The calculations continued until the autoignition process took place. The values of parameters are described in Section 4.

**Fig. 2** Plots of gas temperature versus time, calculated using the first approach (fixed decomposition) (dashed), second approach (coupled solution of the full system of equations) (solid), and the third approach (dynamic decomposition) (dotted). Plots ‘1’, ‘2’ and ‘3’ refer to calculations based on the time steps $10^{-4}$ s, $5 \times 10^{-5}$ s and $10^{-5}$ s respectively. The gas volume is chosen such that if the droplets are fully evaporated without combustion then the equivalence ratio of fuel vapour/air mixture is equal to 4.

**Fig. 3** The same as Fig. 2 but for equivalence ratio.

**Fig. 4** The largest droplet radius versus time, calculated using the first approach (fixed decomposition) (dashed), second approach (coupled solution of the full system of equations) (solid), and the third approach (dynamic decomposition) (dotted). The time step of calculations is taken equal to $10^{-5}$ s.

**Fig. 5** The same as Fig. 1 but for the radius of the largest droplet equal to 17 $\mu$m, gas temperature equal to 780 K, and the gas volume is chosen such that if the droplets are fully
evaporated without combustion then the equivalence ratio of fuel vapour/air mixture is equal to 1 (stoichiometric mixture).

**Fig. 6** Plots of gas temperature versus time, calculated using the first approach (fixed decomposition) (dashed), second approach (coupled solution of the full system of equations) (solid), and the third approach (dynamic decomposition) (dotted). Plots refer to calculations based on the time step $10^{-5}$ s. The gas volume is chosen such that if the droplets are fully evaporated without combustion then the equivalence ratio of fuel vapour/air mixture is equal to 1 (stoichiometric mixture). Values of other parameters are described in Section 4.
NUMBER OF EQUATIONS

TIME [ms]

0.0
0.5
1.0
1.5
2.0
NUMBER OF EQUATIONS

Fig. 5

[ms]

0 1 2 3 4

0 1 2 3 4 5 6 7 8 9 10 11