MFiX: Fractional-Step Method Implementation

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1 Fractional-Step Method

A comprehensive, multiphase computational fluid dynamics (CFD) simulation solves several coupled transport equations including continuity, momentum, species, and energy. Chemical reactions further couple these equations through heats of reaction and rates of formation of products and rates of destruction of reactants. A fractional-step method separates changes attributed to chemical reactions from transport phenomena like convection and diffusion. When the governing equations are split into the transport and reacting components, efficient and independent methodologies can be exploited to solve the different systems. Specifically, discretization of field variable transport equations results in large, sparse matrices which are loosely coupled. These systems are solved in succession using iterative techniques that take advantage of the matrix structure. In contrast, chemical reactions tightly couple field variables locally within the domain (e.g., within a single computational cell) resulting in low-dimensional but dense, nonlinear systems that are better solved using direct integration techniques.

In the following sections, an overview of the mathematical models is provided in the context of the fractional-step method. Next, the systems of ODEs constructed and solved by the stiff chemistry solver is outlined. Lastly, the solution algorithm and details on mapping the ODE solutions into MFiX arrays is reviewed.

2 Mathematical Models

In the fractional-step method, the solution is advanced from t^n to t^{n+1} by solving the transport equations without interphase mass and enthalpy transfer source terms. Specifically, the solution of the previous time step, $\phi_j^n = \phi_j(t^n)$, is advanced to an intermediate solution, $\hat{\phi}_j^{n+1}$. The new time solution, ϕ_j^{n+1}, is then obtained by directly integrating the intermediate state with the chemical reaction source terms.

$$\phi_j^n \xrightarrow{\text{transport}} \hat{\phi}_j^{n+1} \xrightarrow{\text{reactions}} \phi_j^{n+1}$$

The following subsections provide a brief overview of the fluid and continuous and discrete solids mathematical models in MFiX. For each, the full model is described, then the model is separated into the *transport* and *chemical reaction* components. For brevity, the following discussions do not include the momentum equations. The momentum equations do not contain chemical reaction source terms and therefore are included when solving the transport equations.

2.1 Fluid phase model

The fluid phase (gas) species mass and continuity equations are

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g X_{g,n}) + \frac{\partial}{\partial x_i}(\varepsilon_g \rho_g U_{gi} X_{g,n}) = \frac{\partial}{\partial x_i}\left(D_{g,n}\frac{\partial X_{g,n}}{\partial x_i}\right) + R_{g,n} \tag{1}$$

and

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g) + \frac{\partial}{\partial x_i}(\varepsilon_g \rho_g U_{gi}) = \sum_{n=1}^{N_g} R_{g,n} \ . \tag{2}$$

ε_g, ρ_g, $X_{g,n}$ and U_{gi} are the fluid phase volume fraction, material density, n-th species mass fraction, and i-th velocity component, respectively. $D_{g,n}$ is the diffusion coefficient; N_g is the total number of fluid phase species; and $R_{g,n}$ is the rate of production (or consumption) of the n-th fluid species. The energy balance for the fluid phase is

$$\varepsilon_g \rho_g C_{pg} \left[\frac{\partial T_g}{\partial t} + U_{gi}\frac{\partial T_g}{\partial x_i}\right] = -\frac{\partial q_{gi}}{\partial x_i} - \Delta H_g + \mathcal{S}_g^T . \tag{3}$$

where C_{pg} and T_g are the fluid phase specific heat and temperature. The first two terms on the right side represent intra-phase heat conduction and the net heat of reaction for the fluid. The last term is a generalized source term which may include contributions from inter-phase heat transfer and radiative heat transfer among others. An overview of how the heat of reaction is computed and partitioned between phases is provided in [7] in addition to a detailed review of the complete fluid model.

2.1.1 Fluid transport equations

In the absence of phase change and chemical reactions, the fluid equations Eqs. (1)-(3) simplify to

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g X_{g,n}) + \frac{\partial}{\partial x_i}(\varepsilon_g \rho_g U_{gi} X_{g,n}) = \frac{\partial}{\partial x_i}\left(D_{g,n}\frac{\partial X_{g,n}}{\partial x_i}\right) \tag{4}$$

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g) + \frac{\partial}{\partial x_i}(\varepsilon_g \rho_g U_{gi}) = 0 \ , \tag{5}$$

and

$$\varepsilon_g \rho_g C_{pg} \left[\frac{\partial T_g}{\partial t} + U_{gi}\frac{\partial T_g}{\partial x_i}\right] = -\frac{\partial q_{gi}}{\partial x_i} + \mathcal{S}_g^T . \tag{6}$$

For brevity, the fluid momentum equations are omitted; however, it should be noted that the momentum equations are solved along with Eqs. (4)-(6) as part of transport update.

2.1.2 Fluid chemical reaction equations

Neglecting transport effects, the fluid equations reduce to

$$\frac{d}{dt}((\varepsilon\rho)_g X_{g,n}) = R_{g,n} \ , \tag{7}$$

$$\frac{d}{dt}(\varepsilon\rho)_g = \sum_{n=1}^{N_g} R_{g,n} \ , \tag{8}$$

and

$$\frac{dT_g}{dt} = \frac{-\Delta H_g}{(\varepsilon\rho)_g C_{pg}} \ . \tag{9}$$

The apparent density is denoted by $(\varepsilon\rho)_g$ to highlight that this is the term the chemistry solver updates.[1]

2.2 Continuous solids model (TFM)

The TFM m-th solids phase n-th species mass and continuity equations are

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m X_{m,n}) + \frac{\partial}{\partial x_i}(\varepsilon_m \rho_m U_{mi} X_{m,n}) = \frac{\partial}{\partial x_i}\left(D_{m,n}\frac{\partial X_{m,n}}{\partial x_i}\right) + R_{m,n}, \tag{10}$$

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[1] MFiX contains field arrays for fluid volume fraction, ε_g, material density, ρ_g, and apparent density $(\varepsilon\rho)_g = \varepsilon_g \rho_g$.

and

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m) + \frac{\partial}{\partial x_i}(\varepsilon_m \rho_m U_{mi}) = \sum_{n=1}^{N_m} R_{m,n} \ . \tag{11}$$

ε_m, ρ_m, $X_{m,n}$ and U_{mi} are the m-th solids phase volume fraction, material density, n-th species mass fraction, and i-th velocity component, respectively. $D_{m,n}$ is the diffusion coefficient[2]; N_m is the total number of m-th solids phase species; and $R_{m,n}$ is the rate of production (or consumption) of the m-th solids phase n-th species. The energy balance for the m-th solids phase is

$$\varepsilon_m \rho_m C_{pm} \left[\frac{\partial T_m}{\partial t} + U_{mi} \frac{\partial T_m}{\partial x_i} \right] = -\frac{\partial q_{mi}}{\partial x_i} - \Delta H_m + \mathcal{S}_m^T \tag{12}$$

where C_{pm} and T_m are the m-th solids phase specific heat and temperature. The first two terms on the right side represent intra-phase heat conduction and the net heat of reaction. The last term is a generalized source term that may include contributions from inter-phase heat transfer and radiative heat transfer among others. A complete review of the continuous solids model is provided in [7].

2.2.1 TFM solids transport equations

In the absence of phase change and chemical reactions, the m-th solids phase equations Eqs. (10)-(12) simplify to

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m X_{m,n}) + \frac{\partial}{\partial x_i}(\varepsilon_m \rho_m U_{mi} X_{m,n}) = \frac{\partial}{\partial x_i}\left(D_{m,n} \frac{\partial X_{m,n}}{\partial x_i} \right), \tag{13}$$

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m) + \frac{\partial}{\partial x_i}(\varepsilon_m \rho_m U_{mi}) = 0 \tag{14}$$

and

$$\varepsilon_m \rho_m C_{pm} \left[\frac{\partial T_m}{\partial t} + U_{mi} \frac{\partial T_m}{\partial x_i} \right] = -\frac{\partial q_{mi}}{\partial x_i} + \mathcal{S}_m^T. \tag{15}$$

As previously noted, the momentum equations are omitted for brevity; however, the m-th solids phase momentum equations are solved along with Eqs. (13)-(15) as part of the transport update.

2.2.2 TFM solids chemical reaction equations

Neglecting transport effects, the m-th solids phase equations reduce to

$$\frac{d}{dt}((\varepsilon\rho)_m X_{m,n}) = R_{m,n}, \tag{16}$$

$$\frac{d}{dt}((\varepsilon\rho)_m) = \sum_{n=1}^{N_m} R_{m,n}, \tag{17}$$

and

$$\frac{dT_m}{dt} = \frac{-\Delta H_m}{(\varepsilon\rho)_m C_{pm}}. \tag{18}$$

Again, the apparent density for the m-th solids is denoted $(\varepsilon\rho)_m$ to highlight that this is the term the chemistry solver updates.[3].

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[2] By default, the diffusion coefficient for a TFM dispersed phase is zero, therefore Eq. (10) reduces to

$$\frac{\partial}{\partial t}(\varepsilon_m \rho_m X_{m,n}) + \frac{\partial}{\partial x_i}(\varepsilon_m \rho_m U_{mi} X_{m,n}) = R_{m,n}$$

.

[3] MFiX contains field arrays for solids material density, ρ_m, and apparent density, $(\varepsilon\rho)_m$. Solids volume fraction is always computed from these arrays, $\varepsilon_m = (\varepsilon\rho)_m / \rho_m$

2.3 Discrete particle models

MFiX contains three Lagrangian discrete particle models (DPM): DEM (discrete element method) where individual particles are tracked and each collision is resolved [2], Coarse-Grained Particle (CGP) where coarse-grained parcels instead of real particles are tracked and collision forces are calculated using the collision diameter of the computational parcel [4], and PIC (multiphase particle-in-cell) that uses a solids stress to model interactions between statistical groups of particles that share the same physical characteristics (e.g., temperature, density, composition, etc.) [1]. While the equations for motion are very different for DEM, CGP, and PIC, they share nearly identical thermodynamic models. For simplicity and without loss of generality, this discussion refers to DPM elements as particles, although PIC 'particles' are more commonly referred to as parcels or clouds.

The p-th particle n-th species mass and total mass balance are given by

$$\frac{d(m_p X_{p,n})}{dt} = R_{p,n} \tag{19}$$

and

$$\frac{dm_p}{dt} = \sum_{n=1}^{N_p} R_{p,n}. \tag{20}$$

m_p and $X_{p,n}$ are the particle mass and n-th species mass fraction; $R_{p,n}$ is the rate of production (or consumption) of the n-th particle species; and N_p is the number of species that comprise the particle. The p-th particle energy balance is

$$m_p C_{p,p} \frac{dT_p}{dt} = -\Delta H_p + \mathcal{S}_p^T \tag{21}$$

where T_p and $C_{p,p}$ are the particle temperature and specific heat. ΔH_p is the net heat of reaction for the particle, and $\mathcal{S}_p^T$ is a generalized source term that may include inter-phase heat transfer, particle-particle heat transfer, particle-wall heat transfer, and radiation effects[4]. Additional information on the particle thermodynamic models is provided in [5, 6].

2.3.1 DPM solids transport equations

DPM solids mass and species mass are constant in the absence of phase change and chemical reactions; however, the energy balance Eq. (21) reduce to

$$m_p C_{p,p} \frac{dT_p}{dt} = \mathcal{S}_p^T. \tag{22}$$

As with the fluid and TFM solids models, particle position and velocity updates are omitted for brevity; however they are included along with Eq. (22) in the transport update for particles.

2.3.2 DPM solids chemical reaction equations

Considering only chemical reaction sources, the DPM equations for the p-th particle are

$$\frac{d(m_p X_{p,n})}{dt} = R_{p,n}, \tag{23}$$

$$\frac{dm_p}{dt} = \sum_{n=1}^{N_p} R_{p,n}, \tag{24}$$

and

$$\frac{dT_p}{dt} = \frac{-\Delta H_p}{m_p C_{p,p}}. \tag{25}$$

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[4] The MFiX-PIC model does not include particle-particle or particle-wall heat transfer.

3 Implementation

The fractional-step (stiff chemistry) solver implemented in MFIX assumes that the continuous (fluid) phase is always present while continuous and discrete solids are included ‘as-needed’ based on local conditions. Specifically, the stiff solver always integrates fluid quantities[5] but only integrates solids quantities if solids are present in the computational cell.

This section begins by describing the fractional-step implementation for the continuous solids model (TFM) followed by the implementation for the dispersed particle models. Although the implementations are similar there are minor differences in the order in which terms are updated. Then details of the algorithmic implementation are provided, followed by key aspects of mapping the ODE solution into MFiX field variables.

3.1 Continuous solids

The MFiX fractional-step implementation for TFM is illustrated in Figure 1. In general, the workflow is as follows:

1. The fluid momentum and transport equations (4)-(6) and the TFM solids momentum and transport equations (13)-(15) are solved. This advances the fluid and TFM solids field variables from $\phi_j^n = \phi_j(t^n)$ to the intermediate state, $\hat{\phi}_j^{n+1}$.

$$\phi^n \xrightarrow[\substack{fluid\,\&\\ solids}]{transport} \hat{\phi}^{n+1}$$

   An overview of the iterative solution algorithm is provided in [9].

2. Using the intermediate state solutions as the initial conditions, the fluid and TFM solids chemical reaction equations are integrated to complete the time advance from t^n to t^{n+1}.

$$\hat{\phi}^{n+1} \xrightarrow[\substack{fluid\,\&\\ solids}]{reaction} \phi^{n+1}$$

Because the solids material and species densities are typically much larger than those in the fluid phase, Eqs. (16)-(17) are normalized by dividing by the bulk density of solid from the transport equation’s solution, $(\widehat{\varepsilon\rho})_m$. Using a ‘dot’ to indicate the normalized values, e.g., $\dot{(\varepsilon\rho)}_m = (\varepsilon\rho)_m/(\widehat{\varepsilon\rho})_m$, the normalized solids n-th species mass and mass balance equations for chemical reactions are

$$\frac{d}{dt}(\dot{(\varepsilon\rho)}_m X_{m,n}) = \dot{R}_{m,n} \tag{26}$$

$$\frac{d}{dt}(\dot{(\varepsilon\rho)})_m = \sum_{n=1}^{N_m} \dot{R}_{m,n} \tag{27}$$

The coupled ODE system is created by combining the fluid reaction equations (7)-(9) and TFM solids chemical reaction equations (18),(26),(27). An example of the ODE system is provided in (28) for a cell containing M solids phases. The first $2 + N_g$ equations group the fluid apparent density, temperature and N_g species chemical reaction equations. The subsequent M blocks contain $2 + N_m$ equations for each m-th solid phase. If a computational cell does not contain solids, only the fluid equations are included.

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[5] The solver skips cells when the absolute values of all reaction source terms fall below a minimum threshold value.

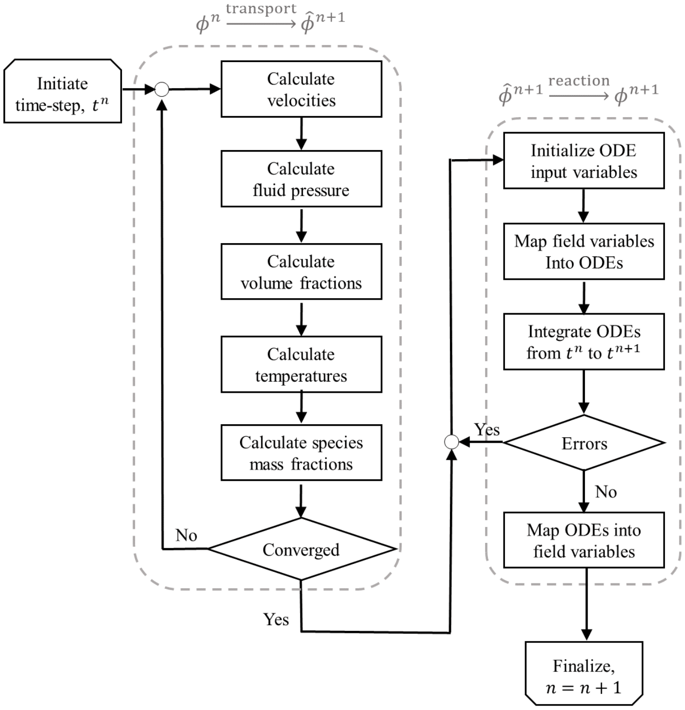

Figure 1: Illustration of solution algorithm in MFiX-TFM with fractional-step method. The grey dashed line (center) encapsulates the algorithm for solving the transport equation. The dashed-dot line (right) outlines the direct linear solver for the reaction equations.

$$\frac{d}{dt}\left[\begin{array}{c} (\varepsilon\rho)_g \\ T_g \\ (\varepsilon\rho)_g X_{g,1} \\ \vdots \\ (\varepsilon\rho)_g X_{g,N_g} \\ \hdashline T_1 \\ \dot{(\varepsilon\rho)}_1 \\ \dot{(\varepsilon\rho)}_1 X_{1,1} \\ \vdots \\ \dot{(\varepsilon\rho)}_1 X_{1,N_1} \\ \hdashline \vdots \\ \hdashline T_M \\ \dot{(\varepsilon\rho)}_M \\ \dot{(\varepsilon\rho)}_M X_{M,1} \\ \vdots \\ \dot{(\varepsilon\rho)}_M X_{M,N_M} \end{array}\right] = \left[\begin{array}{c} \sum_{n=1}^{N_g} R_{g,n} \\ -\Delta H_g/(\varepsilon\rho)_g C_{p,g} \\ R_{g,1} \\ \vdots \\ R_{g,N_g} \\ \hdashline -\Delta H_1/(\varepsilon\rho)_1 C_{p,1} \\ \sum_{n=1}^{N_1} \dot{R}_{1,n} \\ \dot{R}_{1,1} \\ \vdots \\ \dot{R}_{1,N_1} \\ \hdashline \vdots \\ \hdashline -\Delta H_M/(\varepsilon\rho)_M C_{p,M} \\ \sum_{n=1}^{N_M} \dot{R}_{M,n} \\ \dot{R}_{M,1} \\ \vdots \\ \dot{R}_{M,N_M} \end{array}\right] \tag{28}$$

3.2 Discrete particle model

The MFiX fractional-step implementation for DEM is illustrated in Figure 2. The workflow is as follows:

1. The fluid momentum and transport equations (4)-(6) are solve, advancing the fluid field variables from ϕ_j^n to the intermediate state, $\hat{\phi}_j^{n+1}$.

$$\phi_g^n \xrightarrow[fluid]{transport} \hat{\phi}_g^{n+1}$$

2. Next, the fluid and particle chemical reaction equations are integrated. This step completes the fluid advance from time t^n to t^{n+1} and advances particles to an intermediate state.

$$\hat{\phi}_g^{n+1} \xrightarrow[fluid]{reaction} \phi_g^{n+1} \quad \text{and} \quad \phi_p^n \xrightarrow[particles]{reaction} \hat{\phi}_p^{n+1}$$

3. Lastly, particle position, velocity and transport equation (22) are solved to complete the update to time t^{n+1}.

$$\hat{\phi}_p^{n+1} \xrightarrow[particles]{transport} \phi_p^{n+1}$$

This workflow differs from the TFM workflow in that particle positions, velocity and temperature are updated after the chemistry solve. This is due, in part, to how the DPM models are coupled to the fluid model.

Again, because particle material and species densities are typically much larger than those in the fluid phase, Eqs. (23)-(24) are normalized by dividing by particle mass at the start of the time step. Using a 'dot' to indicate the normalized values, e.g., $\dot{m}_p = m_p/m_p(t^n)$, the normalized p-th particle n-th species pass and mass balance equations are

$$\frac{d(m\dot{X}_n)_p}{dt} = \dot{R}_{p,n} \tag{29}$$

and

$$\frac{d\dot{m}_p}{dt} = \sum_{n=1}^{N_p} \dot{R}_{p,n}. \tag{30}$$

The coupled ODE system is created by combining the fluid reaction equations (7)-(9), and particle chemical reaction equations (25),(29),(30). For a cell containing P particles, an example of the ODE system is given by (31) where the first $2{+}N_g$ equations are the fluid apparent density, temperature and N_g fluid species, and the subsequent P blocks contain $2{+}N_p$ equations for each particle whose center resides within the cell. If a cell does not contain any particles, then only the fluid equations are

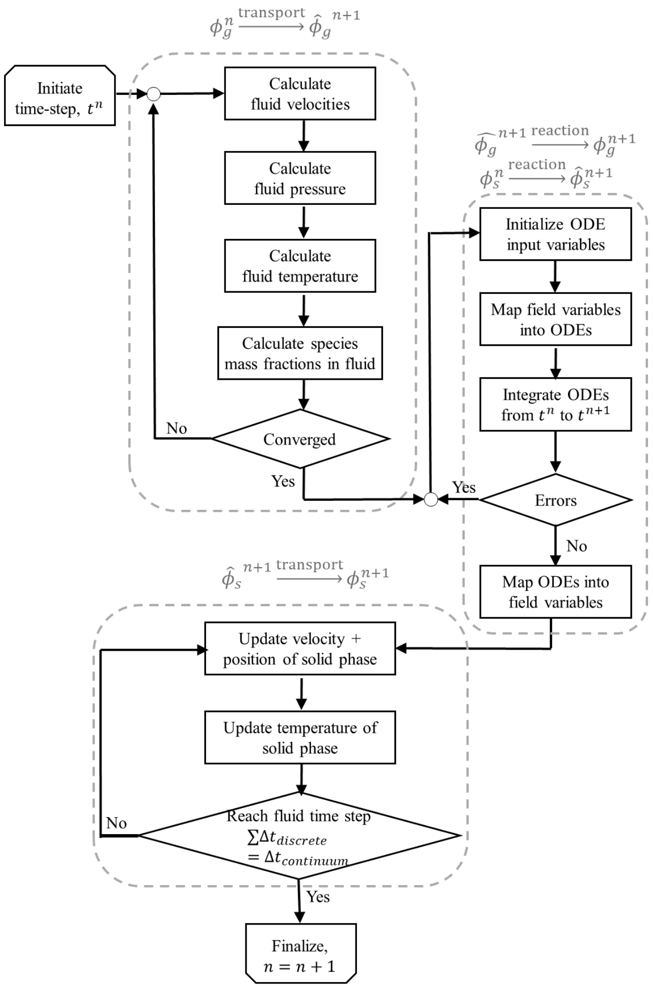

Figure 2: Illustration of solution algorithm in MFiX-DEM with fractional-step method. The grey dashed line (center) encapsulates the algorithm for solving the transport equation. The dashed-dot line (right) outlines the direct linear solver for the reaction equations.

included.

$$\frac{d}{dt}\left[\begin{array}{c} (\varepsilon\rho)_g \\ T_g \\ (\varepsilon\rho)_g X_{g,1} \\ \vdots \\ (\varepsilon\rho)_g X_{g,N_g} \\ \hdashline T_1 \\ \dot{m}_1 \\ \dot{m}_1 X_{1,1} \\ \vdots \\ \dot{m}_1 X_{1,N_1} \\ \hdashline \vdots \\ \hdashline T_P \\ \dot{m}_P \\ \dot{m}_P X_{P,1} \\ \vdots \\ \dot{m}_P X_{P,N_P} \end{array}\right] = \left[\begin{array}{c} \sum_{n=1}^{N_g} R_{g,n} \\ -\Delta H_g/(\varepsilon\rho)_g C_{pg} \\ R_{g,1} \\ \vdots \\ R_{g,N_g} \\ \hdashline -\Delta H_1/m_1 C_{p,1} \\ \sum_{n=1}^{N_1} \dot{R}_{1,n} \\ \dot{R}_{1,1} \\ \vdots \\ \dot{R}_{1,N_1} \\ \hdashline \vdots \\ \hdashline -\Delta H_P/m_P C_{p,P} \\ \sum_{n=1}^{N_P} \dot{R}_{P,n} \\ \dot{R}_{P,1} \\ \vdots \\ \dot{R}_{P,N_P} \end{array}\right] \tag{31}$$

3.3 Algorithm details

A high level overview of the solution methodology is provided in Algo. (1) while Fig. 3 illustrates the workflow along with with an explanation of each subroutine. In general, MFiX populates a 1D array to create the right-hand side (RHS) of the ODE system. During the integration, the 1D array entries are copied back into MFIX field/particle arrays to evaluate user-defined reaction rates which go into forming the left-hand side (LHS) of the ODE system. The ODE integrator, `DLSODA` [3, 8], adjusts the time step size $\Delta\tau$, sub-cycling if necessary, to achieve the desired solution accuracy.

Algorithm 1 MFiX chemistry integration algorithm

```
Copy MFiX field variables into $\mathbf{Y}$, the LHS of Eq. (28)/(31).      ▷ mapMFIXtoODE
$\tau \leftarrow 0$
while $\tau < \Delta t = (t^{n+1} - t^n)$ do                             ▷ Call ODE integrator, DLSODA
    Copy entries of $\mathbf{Y}$ into MFiX field variables.                  ▷ mapODEtoMFIX
    Evaluate user-defined reaction rates                            ▷ USR_RATES/USR_RATES_DES
    Compute $\dot{\mathbf{Y}}$, the RHS of Eq. (28)/(31)                            ▷ STIFF_CHEM_RRATES
    Solve $\frac{d\mathbf{Y}}{dt} = \dot{\mathbf{Y}}$ to advance to $\tau \leftarrow \tau + \Delta\tau$
end while
Copy entries of $\mathbf{Y}$ into MFiX field variables.                      ▷ mapODEtoMFIX
```

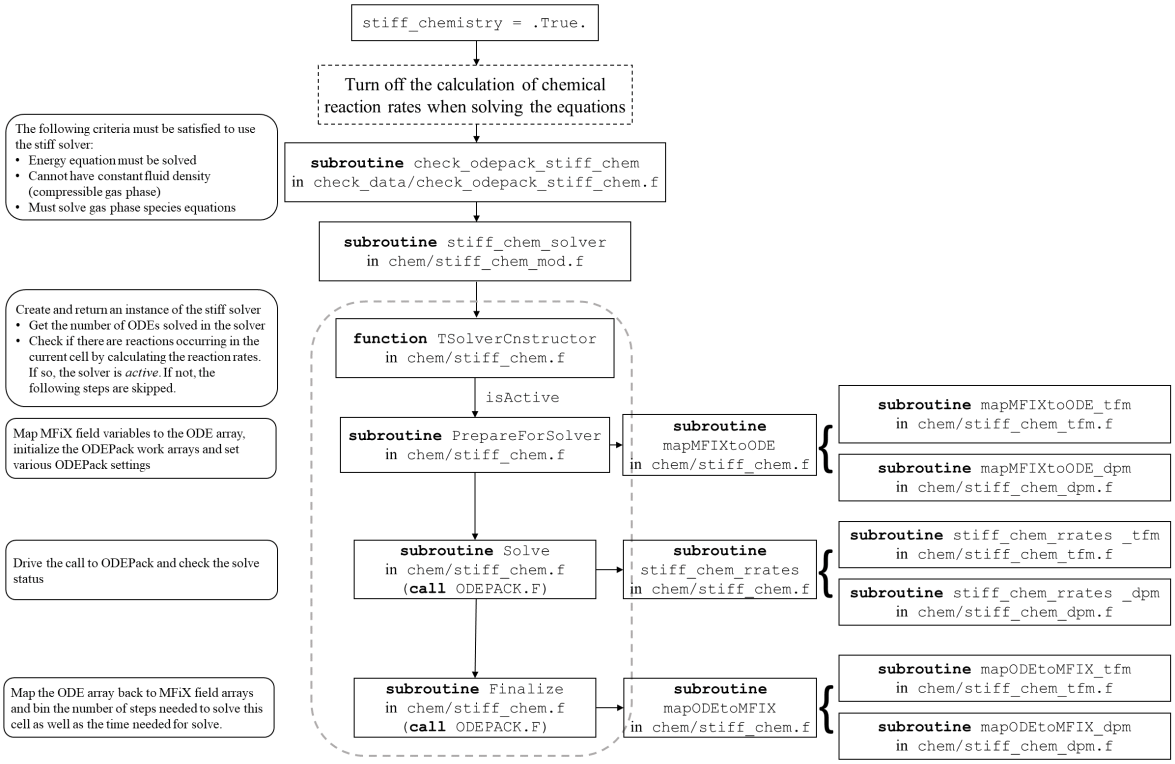

Figure 3: Workflow of subroutines used in the fractional-step method in MFiX. The first column on the left explains the functions of each subroutine/function. The central column outlines the main workflow, with different subroutines for TFM (named with '_tfm') and DEM (named with '_dpm') models shown on the right.

3.4 Mapping between ODEs and field variables

3.4.1 Continuous solids model

The solutions to Eqs. (18),(26),(27) provide updated values for solids temperature, normalized apparent species densities, and normalized apparent density. The temperature is directly copied to the field variable, $T_m = T_m^{ODE}$ whereas the normalized apparent density is multiplied by the intermediate apparent density value.

$$(\varepsilon\rho)_m = (\widehat{\varepsilon\rho})_m \dot{(\varepsilon\rho)}_m^{ODE}$$

The ratio of the normalized apparent species density to normalized apparent density gives the solids species mass fraction.

$$X_{m,n} = \frac{\dot{(\varepsilon\rho X_n)}_m^{ODE}}{\dot{(\varepsilon\rho)}_m^{ODE}}$$

The change in solids mass can be accounted for in one of two ways:

- If the material density is constant, $\rho_m = \rho_m^0$, then the solids volume fraction either increases when there is a net production of solids or decreases when there is a net consumption of solids.

  $$\varepsilon_m = (\varepsilon\rho)_m / \rho_m$$

- If the solids volume fraction is constant, then the material density changes with respect to particle composition,

  $$\rho_m = \rho_m^B \frac{X_{m,I}^B}{X_{m,I}},$$

  where ρ_m^B is the baseline solids density, X_{mI}^B is the baseline mass fraction of the inert solids species, and X_{mI} is the inert species current mass fraction. Details of the mixture solids density model including expanded definitions of the baseline and inert species variables are provided in [7].

The updated fluid volume fraction is computed from the solids volume fractions.

$$\varepsilon_g = 1 - \sum_m \varepsilon_m$$

3.4.2 Discrete particle model

The solutions to Eqs. (25),(29),(30) provide updated values for particle temperature, normalized species mass and total mass, respectively. The temperature is directly copied to the particle array, $T_p = T_p^{ODE}$, while the normalized total mass is multiplied by the starting mass to obtain the updated particle mass.

$$m_p = \dot{m}_p^{ODE} m_p(t^n)$$

The ratio of the normalized species mass and normalized total mass gives the species mass fraction.

$$X_{p,n} = \frac{\dot{(m X_n)}_p^{ODE}}{\dot{m}_p^{ODE}}$$

The change in solids mass can be accounted for in one of two ways:

- If the material density is constant, $\rho_p = \rho_p^0$, then the particle volume, $\mathcal{V}_p$, either increases when there is a net production of solids or decreases when there is a net consumption of solids.

  $$\mathcal{V}_p = m_p / \rho_p$$

  The diameter of the particle is updated from the new volume depending on the assumption of particle shape (e.g. spherical or super-quadric).

- If the solids volume is constant, then the material density changes with respect to particle composition.

$$\rho_p = m_p/\mathcal{V}_p$$

Minor inconsistencies arise in the constant density (changing particle size) case. Specifically, the deposition operation used to compute the Eulerian volume fraction field from Lagrangian particles can spreads (and likely does spread) particle volume across multiple cells. Because the stiff chemistry solver operates on a per-cell basis there is no way to efficiently update the volume fraction field. As a result, the fluid and solids volume fraction fields lag behind the chemistry solve.

3.4.3 Fluid variables

The solutions to Eqs. (7)-(9) provide updated values for the fluid apparent species densities, apparent density and temperature, respectively. The apparent density and temperature are directly stored, $(\varepsilon\rho)_g = (\varepsilon\rho)_g^{ODE}$ and $T_g = T_g^{ODE})$ whereas the ratio of the apparent species densities to apparent density is used to compute the species mass fractions.

$$X_{g,n} = \frac{((\varepsilon\rho)_g X_{g,n})^{ODE}}{(\varepsilon\rho)_g^{ODE}}$$

The updated species mass fractions are used to update the mixture molecular weight,

$$\mathrm{MW}_g = \left(\sum_{n=1}^{N_g} \frac{X_{g,n}}{\mathrm{MW}_n}\right)^{-1},$$

where MW_n is the molecular weight of the n-th species. The fluid material density is computed from the apparent density and volume fraction.

$$\rho_g = (\varepsilon\rho)_g/\varepsilon_g.$$

Lastly, the updated density, temperature, and mixture molecular weight are used to update the fluid pressure using the ideal gas law,

$$P_g = \frac{\rho_g T_g R}{\mathrm{MW}_g},$$

where R is the universal gas constant.

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