On convection-diffusion-reaction and transport-flow problems modelling sedimentation

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Sedimentation of small particles in viscous fluid: unit operation in mineral processing, wastewater treatment, medicine, geophysics, volcanology, and others.

Mathematics needed for the simulation, design and control of processes and equipment.

Macroscopic models (unit-scale, long-time phenomena) ⇒ continuum descriptions of solid/liquid phases.
⇒ nonlinear time-dependent PDEs.
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(De Re Metallica, Freiberg, Saxony, 1556)
Application: Thickeners in Chilean mining industry

- Unit operation of great importance to copper mining in Chile (and elsewhere)
- Purpose of equipment: recovery of process water from flotation tailings (mines mostly located in desert area)
- Inventor: J.V.N. Dorr (1905)
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- Secondary settling tank (SST): coupling with bioreactor, reactive settling/denitrification
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Physics in the oil sands of Alberta

Murray Gray, Zhenghe Xu, and Jacob Masliyah

Alberta’s petroleum reserves are comparable to Saudi Arabia’s, but accessing that oil poses challenges in the physics of fluids and particulates.

Murray Gray is a professor and director of the Centre for Oil Sands Innovation, Zhenghe Xu is a professor and NSERC research chair, and Jacob Masliyah is a university professor emeritus in the department of chemical and materials engineering at the University of Alberta in Edmonton, Canada.

Figure 2. Bitumen production by mining of oil sands. Shovels mine the oil sands, and the trucks carry the mined ore to crushers. The oil-sands lumps are crushed, mixed with warm water and chemicals, and then introduced into a hydrotreatment pipeline. Turbulence in the pipeline liberates the bitumen droplets from solid particles and the droplets become aerated. The flowing slurry is introduced into a large gravity-separation vessel, where the aerated bitumen floats to the top. Coarse sand, fine solids, clays, and some fugitive bitumen sink to the bottom and are usually sent to tailings ponds. The so-called middlings layer is often re-aerated to recover additional bitumen. (Adapted from Barry Bara, Syncrude Canada Ltd.)
Conservation of mass of solids and mixture:

\[ \partial_t \phi + \nabla \cdot (\phi q + \phi (1 - \phi) v_r) = 0, \quad \nabla \cdot q = 0. \]

\( \phi \): local solids volume fraction, \( v_s, v_f \): solids/fluid phase velocity; 
\( v_r := v_s - v_f, \quad q := \phi v_s + (1 - \phi) v_f \):

- Constitutive assumption for \( v_r \) \( \Rightarrow \) in 1-d model is closed
- In 2-d or 3-d, additional eqns necessary so that \( q \) is determined
- Kinematic sedimentation model\(^1\): assume \( v_r \uparrow = v_r(\phi) \)
- In 1-d, closed cylindrical column: scalar conservation law (SCL)

\[ \partial_t \phi - \partial_x f(\phi) = 0, \quad f(\phi) = \phi v_{hs}(\phi), \quad (SCL) \]

\[ v_{hs}(\phi) = (1 - \phi) v_r(\phi) = v_{Stokes}(1 - \phi)^{n_{RZ}}, \quad v_{Stokes} = g d^2 \frac{\rho_s - \rho_f}{18 \mu_f}. \]

\(^1\)Steinour Ind. Engrg. Chem. (1944); Kynch Trans. Farad. Soc. (1952)
Balance equations and a simple model of batch settling

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Jump conditions, solutions for batch settling

- Rankine-Hugoniot condition: if $\phi^+(t)$, $\phi^-(t)$ are solution values adjacent to a curve $t \mapsto x_d(t)$, then

$$- \frac{dx_d}{dt} = S(\phi^-, \phi^+) := \begin{cases} 
\frac{f(\phi^+) - f(\phi^-)}{\phi^+ - \phi^-} & \text{if } \phi^+ \neq \phi^-; \\ f'(\phi^-) & \text{if } \phi^+ = \phi^-.
\end{cases}$$

(RH)

- A discontinuity is said to be admissible if

$$S(\phi^-, \phi^+) \leq S(\phi^-, \phi) \quad \text{for all } \phi \text{ between } \phi^- \text{ and } \phi^+. \quad \text{(EJ)}$$

- Settling of homogeneous suspension\(^2\): pair of Riemann problems:
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Continuous sedimentation: PDE with rough coefficients

- For constant cross-sectional area $A$,

\[
\frac{\partial t}{\partial \phi} + \frac{\partial z}{z} \left( \frac{Q(z,t)}{A} \phi + \gamma(z)f(\phi) \right) = \frac{\partial z}{z} \left( \gamma(x) \frac{\partial z}{D(\phi)} \right) + \delta(z) \frac{Q_f}{A} (\phi - \phi_f),
\]

- PDE is strongly degenerate: there is a critical concentration $\phi_c$ such that

\[
D(\phi) = 0, \phi \leq \phi_c; \quad D'(\phi) > 0, \phi > \phi_c.
\]

- Discontinuous flux due to diverging bulk flows, where $Q_f = Q_u - Q_e$:

\[
Q(z,t) = \begin{cases} 
-Q_e(t) & \text{for } z \leq 0, \\
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  - sediment compressibility
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**Conservation law with discontinuous flux**

For \( D \equiv 0 \) and stationary bulk flows,

\[
\partial_t \phi + \partial_z g(\phi, z) = 0,
\]

\[
g(\phi, z) = \begin{cases} 
-\frac{Q_e}{A}(\phi - \phi_f), & z < -H, \\
-\frac{Q_e}{A}(\phi - \phi_f) + f(\phi), & -H < z < 0, \\
\frac{Q_u}{A}(\phi - \phi_f) + f(\phi), & 0 < z < B, \\
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- Model has partly motivated well-posedness and numerical analysis for

\[
\begin{cases} 
\partial_t u + \partial_x F(u, x) = 0, \quad x \in \mathbb{R}, \quad t > 0, \\
u(x, 0) = u_0(x), \quad x \in \mathbb{R};
\end{cases}
\]

\[
F(u, x) = \begin{cases} 
f(u), & x \geq 0, \\
g(u), & x < 0.
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\]

- \( f(u_+(t)) = g(u_-(t)) \) across \( x = 0 \) can be satisfied in multiple ways.
- Solution concept depends on model (e.g., vehicular traffic, flow in heterogenous porous media). Well-posedness is not a straightforward limit case of theory of PDE with smooth coefficients.
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- **Contributions include**: Mochon 87; Gimse & Risebro 92; Diehl 95–; Ostrov 99–; Karlsen, Risebro & Towers 03; Seguin & Vovelle 03; Adimurthi, Veerappa Gowda & Mishra 05, Panov 05–; Audusse & Perthame 05; Bachmann & Vovelle 06; Andreianov, Karlsen & Risebro 11, Andreianov & Mitrović 15

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- For **continuous sedimentation model** with $D \neq 0$, well-posedness, convergence of numerical schemes established\(^3\).

- Model widely accepted, extensions to reactive settling, applications in mineral processing and wastewater treatment (water resource recovery).

\(^3\)B, Karlsen & Towers *SIAP* (2005)
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Outline of presentation

- Nonlinear coefficients must be calibrated
  \[ \Rightarrow \text{inverse problem (model function identification from data)} \]
  **Topic 1**: Flux identification from settling in a cone

- Applications to wastewater treatment plants involve chemical reactions
  \[ \Rightarrow \]
  **Topic 2**: Modelling sedimentation with reactions ("reactive settling")

- New methods for the simulation in multiple space dimensions
  **Topic 3**: On coupled transport-flow problems
Nonlinear coefficients must be calibrated
⇒ inverse problem (model function identification from data)
Topic 1: Flux identification from settling in a cone

Applications to wastewater treatment plants involve chemical reactions ⇒
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**Topic 3**: On coupled transport-flow problems
Topic 1: Flux identification from settling in a cone

- Settling in a vessel with variable cross-sectional area $A(x)$ (disregarding compressibility, wall effects):

$$\frac{\partial}{\partial t} (A(x)\phi) - \frac{\partial}{\partial x} (A(x)f(\phi)) = 0,$$

$$\phi(x, 0) = \phi_0 \quad \text{for } 0 < x < 1,$$

$$\phi(0^+, t) = \phi_{\text{max}} = 1, \quad \phi(1^-, t) = 0 \quad \text{for } t > 0$$

- $f \in C^2, f(0) = f(1) = 0,$ single max $\phi^M, \phi_{\text{infl}} \in (\phi^M, 1]$ 

- “Imhoff cone”:

- $A(x) = \left(\frac{p + qx}{p + q}\right)^{1/q}, p, q \geq 0;$

- full cone: $p = 0, q = 1/2.$
Topic 1: Flux identification from settling in a cone

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"Imhoff cone":
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  $$\partial_t (A(x)\phi_t) - \partial_x (A(x)f(\phi)) = 0,$$
  
  $$\phi(x,0) = \phi_0 \quad \text{for} \quad 0 < x < 1,$$
  
  $$\phi(0^+, t) = \phi_{\text{max}} = 1, \quad \phi(1^-, t) = 0 \quad \text{for} \quad t > 0$$

- $f \in C^2$, $f(0) = f(1) = 0$, single max $\phi^M$, $\phi_{\text{infl}} \in (\phi^M, 1]$ “Imhoff cone”:

- $A(x) = \left(\frac{p + qx}{p + q}\right)^{1/q}$, $p, q \geq 0$;

- full cone: $p = 0, \ q = 1/2$. 

- **Flux identification**

- **Reactive settling**

- **Coupled flow-transport problems**

- **Conclusions**
New contribution

- Explicit entropy solutions\(^4\) to (IBVP): method of characteristics (\(\neq\) iso-\(\phi\)-curves), numerical approximation of curved shocks.
- For concave-convex \(f\): 3 different solutions, in dependence of \(\phi_0\).
- Suspension-supernate interface in a cone appeals to a range of \(\phi\)-values \(\Rightarrow\) new method of efficient flux identification\(^5\).
- Inverse problem (IP): given \([t_{\text{start}}, t_{\text{end}}] \ni t \mapsto h(t)\), find the portion of \(\phi \mapsto f(\phi)\) corresponding to the interval of adjacent \(\phi\)-values.

\(^4\) B, Careaga & Diehl SIAP (2017)
New contribution

- Explicit entropy solutions\(^4\) to (IBVP): method of characteristics (≠ iso-$\phi$-curves), numerical approximation of curved shocks.
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\textsuperscript{4}B, Careaga & Diehl SIAP (2017)
Entropy solutions and characteristics for model problem

**Definition (Entropy solution of (IBVP))**

A function \( \phi = \phi(x, t) \) is an entropy solution if \( \phi \in C^1 \) with the exception of finitely many curves \( x_d(t) \), where \( \phi(x_d(t)^\pm, t) \) satisfy (RH) and (EJ).

- Quasilinear form of PDE: \( \partial_t \phi - f'(\phi) \partial_x \phi = \frac{A'(x)}{A(x)} f(\phi) \). For characteristics emanating from \( (x, t, \phi) = (\xi, \tau, \varphi) \): solve

  \[
  \begin{aligned}
  X'(t) &= -f'(\Phi), \quad t > \tau; \\
  X(\tau) &= \xi, \\
  \Phi'(t) &= \frac{A'(X)}{A(X)} f(\Phi) > 0, \quad t > \tau; \\
  \Phi(\tau) &= \varphi,
  \end{aligned}
  \]

- For \( A(x) = \left( \frac{p+qx}{p+q} \right)^{1/q} \), we get the characteristic system

  \[
  \frac{t - \tau}{p + qx} = f(\phi) \int_{\phi_0}^{\phi} \frac{d\Phi}{f(\Phi)^{1+q}}, \quad \frac{f(\phi)}{f(\varphi)} = \left( \frac{p + q\xi}{p + qx} \right)^{1/q}. \tag{CS}
  \]

  Special case starting from \( (x, t, \phi) = (\xi, 0, \phi_0) \):

  \[
  \psi(x, t) := \frac{t}{p + qx} = f(\phi)^q \int_{\phi_0}^{\phi} \frac{d\Phi}{f(\Phi)^{1+q}} =: Q(\phi) \Rightarrow \phi = Q^{-1}(\psi(x, t)).
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  **(CS)**

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  \]
Entropy solutions \((p > 0)\)

- Cases of \(\phi_0\) for concave-convex \(f\): low (L), medium (M), high (H):

\[
\begin{align*}
\phi_0 & \leq \phi_{\text{max}}^* & \phi_{\text{max}}^* & \leq \phi_0 & \leq \phi_{\text{infl}} & \phi_0 & \geq \phi_{\text{infl}}
\end{align*}
\]

**Theorem (Main result, B, Careaga & Diehl 17)**

1. (IBVP) has three qualitatively different, piecewise smooth entropy solutions formed by characteristics and curved trajectories of entropy-satisfying shocks and contact discontinuities.
2. The descending shock \(h(t)\) is strictly convex for \(0 < t < t_3\).
3. A rising shock \(b(t)\) may form and meet, or not meet, \(h(t)\).
4. The solution is continuous below \(h(t)\) in certain cases for a full cone.
For the purpose of illustration, we use \( f(\phi) = \phi(e^{-rv\phi} - e^{-rv\phi_{\text{max}}}) \).

Parameters: \( r_V = 4, \phi_0 = 0.04, q = 1/2, p = 1/18 \).
Solutions, Cases L, M, H, $p > 0$

- $r_V = 4,$  
  $\phi_0 = 0.1,$  
  $q = 1/2, p = 1/3$

- $r_V = 5,$  
  $\phi_0 = 0.12,$  
  $q = 1/2, p = 1/6$

- $r_V = 4.7,$  
  $\phi_0 = 0.43,$  
  $q = 1/2, p = 9.5$

From the upper discontinuity $h(t)$ and $\phi_h = \phi(h^-(t), t)$:

$$f(\phi_h(t)) = -h'(t)\phi_h(t), \quad 0 \leq t \leq t_{2.5},$$

$$\psi(h(t), t) = Q(\phi_h(t)), \quad 0 \leq t \leq t_{2.5}. $$
Solution, Case M, $p = 0$

- If $\frac{Q'(\phi_{infl})}{qf(\phi_{infl})^{q-1}} > 0$, then $\phi$ is continuous for $0 \leq x \leq h(t)$.
- $f(\phi)$ can be reconstructed for $\phi \in [\phi_0, \phi_{max}]$ for $p = 0$.
- Choose here $r_V = 4.7$, $\phi_0 = 0.43$, $q = 1/2$, $p = 0$:

This case is of interest for flux identification.
The inverse problem

Theorem (Solution of the inverse problem)

Assume \( p \geq 0, q > 0 \), and that \( \phi_0 \) and \( x = h(t), 0 \leq t < t_{2.5}, \) are known. Then (IP) has the parametrized solution

\[
\begin{pmatrix}
\phi \\
\phi h'(t)
\end{pmatrix} = \phi_0 \frac{(p + q)^{1+1/q}}{(p + qh(t))^{1/q}(p + q\eta(t))} \begin{pmatrix} 1 \\
-h'(t)
\end{pmatrix}, \quad 0 \leq t \leq t_{2.5},
\]

where \( \eta(t) := h(t) - th'(t) \), or the explicit solution

\[
f(\phi) = -\phi h' \left( \sigma^{-1} \left( \frac{\phi_0 (p + q)^{1/q+1}}{\phi} \right) \right), \quad \phi_0 \leq \phi \leq \phi_h(t_{2.5}),
\]

where \( s(t) := (p + qh(t))^{1/q+1} \) and \( \sigma(t) := s(t) - \frac{qt}{q+1} s'(t) \).

Both formulas presuppose \( h'(t) < 0 \) and \( h''(t) > 0 \).
Application to discrete data

- Formulate (IP) as a least squares problem for $h$. Approximate data $(t_i, h(t_i)), i = 1, \ldots, N$, by $h_{\text{spline}}$:

$$h_j(t) = a_j t^3 + b_j t^2 + c_j t + d_j, \quad j = 1, \ldots, J,$$

i.e. $h_{\text{spline}} = h_j$ on the $j$-th subinterval.

- We impose $h_{\text{spline}} \in C^2, h'_{\text{spline}} < 0, h''_{\text{spline}} > 0$.

- Solving for coefficients $p$ leads to constrained least squares (quadratic programming) problem:

\[
\begin{align*}
\text{minimize} & \quad J(p) = (Qp - h)^T(Qp - h) \\
\text{subject to} & \quad Rp = 0, \quad Mp \leq b.
\end{align*}
\]

- Alternatively, solve a least squares problem for $s$. 
Example 1: synthetic data in cone

- Parameters: $r_V = 5$, $\phi_0 = 0.1$

$h$-curve: 5 subintervals

![h-curve graph]

flux: 5 subintervals

![flux graph 1]

flux: 20 subintervals

![flux graph 2]

$s$-curve: 5 subintervals

![s-curve graph]

flux: 10 subintervals

![flux graph 3]

flux: 40 subintervals

![flux graph 4]
Example 2: using experimental data in a cone

- Material: activated sludge, Västeras WWTP, Sweden

Experimental setup

Measurements

Reconstructed portion

Complete flux

Re-simulation

Re-simulation (zoom)
**Topic 2: Reactive settling**

- Concentration vectors:
  - Particulate components $C(z,t)$
  - Substrate components $S(z,t)$
- Feed inputs: $C_f(t), S_f(t)$
- Volumetric flows:
  - Feed $Q_f(t)$ (known)
  - Underflow $Q_u(t)$ (known)
  - Effluent $Q_e(t, C, S)$
- Include Activated Sludge Model (biokinetic model) at every depth $z$
- Modelling idea: hindered and compressive settling depends on total particulate concentration (flocculated biomass) $X$

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Concentrations, percentages and other ingredients

- **Solid phase**: concentration: $X$, velocity: $v_X$, density: $\rho_X = \text{const.}$,

\[ C = p_X X = \left( p_X^{(1)}, \ldots, p_X^{(k_X)} \right)^T X. \]

- **Liquid phase**: concentration: $L$, velocity: $v_L$, density: $\rho_L = \text{const.}$,

\[ p_L L = \left( p_L^{(1)}, \ldots, p_L^{(k_L)} \right)^T L = \left( S^{(1)}, \ldots, S^{(k_L-1)}, W \right)^T \]

\[ \begin{array}{c}
\Sigma = 1 \\
\text{water}
\end{array} = \text{S} \]

- $R_X(C, S)$, $R_L(C, S)$: reaction terms of activated sludge model

- **Constitutive equation for relative velocity**:

\[ v_X - v_L = v_{\text{rel}} = \frac{\gamma(z)}{1 - X/\rho_X} \left( f_b(X) - \partial_z D(X) \right), \]

\[ f_b(X) = X v_{hs}(X): \text{batch settling, } \partial_z D(X): \text{sediment compressibility:} \]

\[ D(X) = \int_0^X \bar{d}(s) \, ds, \quad d(X) = \frac{v_{hs}(X)}{g(1 - \rho_L/\rho_X)} \sigma'(X) \left\{ \begin{array}{ll}
= 0 & \text{for } X \leq X_c, \\
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\end{array} \right. \]
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  \]
Final form of model PDEs in “solvable order”

- Balance equations:

\[
\begin{align*}
\partial_t X + \partial_z F_X &= \delta(z) \frac{X_f Q_f}{A} + \gamma(z) \tilde{R}_X, \\
\partial_t (p_X X) + \partial_z (p_X F_X) &= \delta(z) \frac{p_{X,f} X_f Q_f}{A} + \gamma(z) R_X, \\
L &= \rho_L (1 - X/\rho_X), \\
\partial_t (\bar{p}_L L) + \partial_z (\bar{p}_L F_L) &= \delta(z) \frac{\bar{p}_{L,f} L_f Q_f}{A} + \gamma(z) \bar{R}_L, \\
p_L^{(k_L)} &= 1 - (p_L^{(1)} + \cdots + p_L^{(k_L-1)}),
\end{align*}
\]

- \( \tilde{R}_X := R_X^{(1)} + \cdots + R_X^{(k_X)} \); \( \bar{p}_L \) = first \( k_L - 1 \) components of \( p_L \),

\[
F_X = X q + \gamma(z) (f_b(X) - \partial_z D(X)), \quad F_L = \rho_L (q - F_X/\rho_X)
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\[ L = \rho_L (1 - X/\rho_X), \]
\[ \partial_t (\tilde{p}_L L) + \partial_z (\tilde{p}_L F_L) = \delta(z) \frac{\tilde{p}_L f L_f Q_f}{A} + \gamma(z) \tilde{R}_L, \]
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- Strong coupling via the bulk velocity; here \( q = q(z, t) = Q(z, t)/A. \)
**Numerical scheme**

- **Marching formula**, \([\Delta F^n_X]_j := F^n_{X,j+1/2} - F^n_{X,j-1/2} :\)

\[
\frac{X^{n+1}_j - X^n_j}{\Delta t} = - \frac{[\Delta F^n_X]_j}{\Delta z} + \delta_{j,jf} \frac{X^n_f Q^n_f}{A\Delta z} + \gamma_j \tilde{R}^n_{X,j}
\]

- **\(F^n_{X,j+1/2} := B^n_{j+1/2} + G^n_{j+1/2} - J^n_{j+1/2} :\) upwind formulas, Godunov scheme, second differences**

- **Percentage propagation (formula for \(P^n_{L,j+1}\) similar):**

\[
\frac{P^{n+1}_{X,j} X^{n+1}_j - P^n_{X,j} X^n_j}{\Delta t} = - \frac{[\Delta P^n_X F^n_X]_j}{\Delta z} + \delta_{j,jf} \frac{P^n_{X,f} X^n_f Q^n_f}{A\Delta z} + \gamma_j R^n_{X,j}
\]

\(P^n_{X,j+1/2} := \begin{cases} 
P_{X,j+1}, & F^n_{X,j+1/2} \leq 0, \\
P_{X,j}, & F^n_{X,j+1/2} > 0. 
\end{cases}\)
Invariant region principle

Theorem

If the CFL condition of type

$$\Delta t \left( A + \frac{B}{\Delta z} + \frac{C}{\Delta z^2} \right) \leq 1$$

and certain technical assumptions are satisfied, then the numerical scheme satisfies the following for all layers $j$ and time points $t_n$:

$$0 \leq X^n_j \leq X_{\text{max}}, \quad L^n_j > 0, \quad 0 \leq P^n_{X,j}, P^n_{L,j} \leq 1,$$

$$\sum_{i=1}^{k_X} P^{(i),n}_{X,j} = \sum_{i=1}^{k_L} P^{(i),n}_{L,j} = 1.$$
Numerical simulations: components and reactions

- Model of denitrification\(^7\): bound nitrogen $\rightarrow$ free $N_2$. Components:

  \[
  k_X = 2:
  \begin{cases}
  X_{\text{OHO}} & \text{ordinary heterotrophic organisms}, \\
  X_U & \text{undegradable organics}, \\
  \end{cases}
  \]
  \[
  k_L - 1 = 3:
  \begin{cases}
  S_{\text{NO}_3} & \text{nitrate}, \\
  S_S & \text{readily biodegradable substrate}, \\
  S_{\text{N}_2} & \text{nitrogen}.
  \end{cases}
  \]

- Reaction terms ($C = (X_{\text{OHO}}, X_U)^T$, $S = (S_{\text{NO}_3}, S_S, S_{\text{N}_2})^T$):

  \[
  R_X = X_{\text{OHO}}\left(\mu(S) - b, f_P b\right),
  \]
  \[
  R_L = X_{\text{OHO}}\left(-\frac{1 - Y}{2.86Y}\mu(S), -\frac{1}{Y}\mu(S) + (1 - f_P)b, \frac{1 - Y}{2.86Y}\mu(S), 0\right)^T,
  \]
  \[
  \mu(S) := \mu_{\text{max}} \frac{S_{\text{NO}_3}}{K_{\text{NO}_3} + S_{\text{NO}_3}} \frac{S_S}{K_S + S_S} \quad \text{(growth rate function)}.
  \]

Model functions and scenarios

- Hindered settling and compression, where $X_c = 5 \text{ kg/m}^3$:
  \[ v_{hs}(X) = \frac{v_0}{1 + (X/\bar{X})^{\bar{r}}}, \quad \sigma_e(X) = \begin{cases} 
  0 & \text{for } X < X_c, \\
  \alpha(X - X_c) & \text{for } X > X_c,
  \end{cases} \]

- Simulations start from steady state.
- Variations of feed variables in Example 3:

- Spatial discretization always $N = 2430$
Example 3

(a) $X(z, t)$ [kg/m$^3$]
(b) $X_{OHO}(z, t)$ [kg/m$^3$]
(c) $X_{U}(z, t)$ [kg/m$^3$]
(d) $S_{NO_3}(z, t)$ [kg/m$^3$]
(e) $S_{S}(z, t)$ [kg/m$^3$]
(f) $S_{N_2}(z, t)$ [kg/m$^3$]
(g) $W(z, t)$ [kg/m$^3$]
Example 3: numerical error

- Snapshots at different times, “eyeball norm”:

  - (a) $X_{\text{OHO}}(z, t)$ [kg/m$^3$]
  - (b) $X_{\text{OHO}}(z, t)$ [kg/m$^3$]
  - (c) $X_{\text{OHO}}(z, t)$ [kg/m$^3$]
  - (d) $S_{N_2}(z, t)$ [kg/m$^3$]
  - (e) $S_{N_2}(z, t)$ [kg/m$^3$]
  - (f) $S_{N_2}(z, t)$ [kg/m$^3$]

- According to design, scheme is formally first-order accurate; in presence of discontinuities smaller rates
Topic 3: Coupled flow-transport problems

- Wish to simulate sedimentation processes in geometries like:
  - inclined channel
  - axisymmetric CT

- Volume average velocity $q$ in

$$\phi_t + \text{div}(\phi q + \phi(1 - \phi)v_r(\phi, \nabla \phi)) = 0, \quad \text{div} q = 0$$

not determined ⇒ need additional equations for motion of mixture
Coupled transport-flow problem

- **Incompressible mixture**:\(^8\)\(^9\):

\[
\begin{align*}
\partial_t \phi + \text{div} \left( \phi \mathbf{q} - f(\phi) \mathbf{k} \right) &= \text{div} \left( \kappa(\phi) \nabla \phi \right), \\
\partial_t \mathbf{q} + \mathbf{q} \cdot \nabla \mathbf{q} - \frac{1}{\rho} \text{div} \left( \mu(\phi) \varepsilon(\mathbf{q}) - p \mathbf{I} \right) &= Q(\phi) (\partial_t \mathbf{v}_r + \mathbf{q} \cdot \nabla \mathbf{v}_r) \\
&+ Q(\phi) \mathbf{v}_r \cdot \nabla \mathbf{q} + g \mathbf{k}, \\
\text{div} \mathbf{q} &= 0,
\end{align*}
\]

(CFTP)

- \(\rho = \phi \rho_X + (1 - \phi) \rho_L\): local density of mixture, \(\mathbf{k}\): vector pointing into direction of gravity

- Other functions:

\[
Q(\phi) = \frac{\rho_X - \rho_L}{\rho} \phi (1 - \phi), \quad \kappa(\phi) := \frac{D'(\phi)}{\rho_X}, \quad \mu(\phi) := \frac{1}{(1 - \phi)^3}.
\]

- Primal unknowns: velocity \(\mathbf{q}\), solids concentration \(\phi\), pressure \(p\).

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\(^8\)B, Wendland & Concha ZAMM (2000)  
\(^9\)Ruiz-Baier & Lunati JCP (2016)
Mixed formulation

- Find the Cauchy fluid pseudo-stress $\sigma$, the velocity $q$, and the volume fraction $\phi$ satisfying

\[
\frac{1}{\mu(\phi)} \sigma^d = \nabla q, \quad \partial_t q - \text{div}\sigma = f\phi, \quad \text{div} q = 0 \quad \text{in} \ \Omega,
\]

\[
\tilde{\sigma} = \kappa(\phi) \nabla \phi - \phi q + b(\phi)k, \quad \partial_t \phi - \text{div}\tilde{\sigma} = g \quad \text{in} \ \Omega.
\]

Boundary conditions:

\[
q = q_D, \quad \phi = \phi_D \quad \text{on} \ \Gamma_D; \quad \sigma \nu = 0, \quad \tilde{\sigma} \cdot \nu = 0 \quad \text{on} \ \Gamma_N,
\]

along with initial data $q(0) = q_0, \ s(0) = s_0$ in $\Omega \times \{0\}$.

- Problems with these ingredients have successfully been simulated numerically by many techniques (Alvarez, Gatica & Ruiz-Baier 15—).

- Study of mathematical properties of (CFTP) and the rigorous analysis of discretizations is still an open problem in the general case.

- Available treatments presuppose non-degeneracy of the diffusion term.
Finite volume element (FVE) schemes

- **Finite volume (FV)-based discretizations**: suggested when convection in diffusive transport equation is dominant.

- **Finite element (FE) formulations**: more suitable for error analysis by energy arguments and mixed formulations.

- **Finite-volume-element (FVE) schemes** retain properties of both FV and FE methods. Their construction hinges on defining fluxes across element boundaries defined on a dual partition of the domain (Bank & Rose 87).

- Applications to incompressible flows: Quarteroni & Ruiz-Baier 11, Wen, He & Yang 13 Kumar & Ruiz-Baier 15)

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Example 4: axisymmetric secondary settling tank

Tank of Eindhoven WWTP (courtesy Biomath, Ghent U., Belgium)

- $q_{in} = (0, 0.17)^T$, $\phi_{in} = 0.08$, $q_{out} = (0, -0.0000015)^T$ $\Gamma_{out}$, constant pressure profile imposed at the overflow $\Gamma_{ofl}$
- zero-flux BCs for $\phi$, no-slip on $\partial\Omega$ (with exception of $r = 0$).
- $\sigma_e(\phi) = (\sigma_0 \alpha/\phi_c^\alpha) \phi^{\alpha-1}$, $\sigma_0 = 0.22$ Pa, $\alpha = 5$, $\beta = 2.5$, $\rho_L = 998.2$ kg/m$^3$, $\rho_X = 1750$ kg/m$^3$, $\phi_c = 0.014$, $\tilde{\phi}_{max} = 0.95$, $v_\infty = 0.0028935$ m/s, $g = 9.8$ m/s$^2$, and $D_0 = 0.0028935$ m$^2$/s.
- Primal formulation$^{11}$: 96772 triangles, 48387 vertices, $\Delta t = 3$ s

$^{11}$B, Kumar & Ruiz-Baier JCP (2015)
Example 4: concentration

Concentration $\phi$ at $t = 100$ s—5000 s—50000 s—100000 s

Figure showing concentration plots at different time intervals.
Example 4: pressure and velocities

$t = 100\ s$

$t = 5000\ s$

$t = 50000\ s$

$t = 100000\ s$
Example 4: a posteriori error estimation

- **Mesh adaptivity** guided by a posteriori error estimates useful for sedimentation-consolidation problems (concentration of computational effort on zones of interest)
- Efficient and reliable residual-based a posteriori error estimators for augmented mixed–primal FE schemes for stationary versions of model, recently proposed\(^\text{12}\)
- Lowest-order mixed-primal scheme\(^\text{13}\)
- Backward Euler method for time discretization, $\Delta t = 5$ s; $t_{\text{final}} = 12000$ s.

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Numerical results: snapshots at $t = 4000\,\text{s}$ and $t = 12000\,\text{s}$
Conclusions

- **Topic 1:** (IP) can be solved using the equations that we found for $h$ in the construction of the entropy solution.

- To obtain even better approximation from experimental data we require the identification of the convexity/concavity of $f$.

- Formulation related to the cross-sectional area should be revised.

- **Topic 2:** Results illustrate complex flow-reaction processes that involve independent time scales (transport versus reaction).

- Description is still incomplete; e.g., for more realism, formation of $N_2$ bubbles should be taken into account.

- **Topic 3:** Most important transport and flow features are described realistically.

- Strong ellipticity and monotonicity are still fundamental to derive and analyze numerical methods. An open research problem is the construction and analysis of methods for the strongly degenerate case.
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Ongoing work includes:

- **Polydisperse suspensions**: assumption of $N$ segregating particle species leads to $N \times N$ systems of conservation laws:
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Common flux vectors $f$ proposed in literature have Jacobians that are low-rank perturbations of diagonal matrix: eigenvalue estimates, spectral methods feasible; possibly diffusion terms

- **Related unit operation**: flotation column (attachment of hydrophobic particles to gas bubbles)

- **Future applications**: flows with mass transfer, non-constant densities; leaching, washing (hydrometallurgy), countercurrent decantation

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