# Towards a multiscale strategy for modeling high-pressure flow of carbon dioxide for sequestration

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## Background

- $CO_2$ storage and gas/oil recovery technology is advancing rapidly
- Transport (*the missing link* [19]), storage and recovery modeling capability is increasingly a rate-limiting factor for system improvement
- Two key physical modeling issues are
  -Reservoir dynamics
  -Wellbore hydraulics (this project)
- Wellbore flow is:
  -turbulent
  -multiphase and/or multicomponent
  -dominated by distinctive flow patterns
- Current system modeling approaches are empirical and dont adequately treat
  -multi-component flow (e.g, water, $CO_2$, or other combustion products)
  -transients

Current CFD methods do not capture the crucial effects of multiphase microphysics on flow pattern selection!

Advanced $CO_2$ storage/gas/oil recovery techniques pose wellbore flow modeling challenges

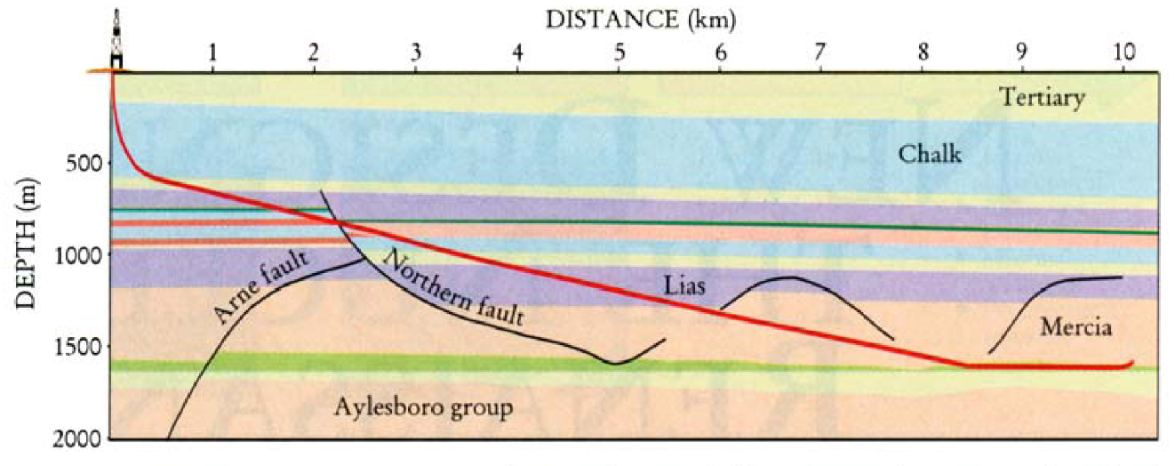


**FIGURE 3. EXTENDED-REACH WELL** in the Wytch Farm field on the southern coast of England. The drilling rig is on shore, but most of the well (red) is under the sea. The well reaches a depth of 1.5 km before it terminates in sherwood sandstone, and has a lateral extent of about 10 km.

Figure taken from Physics Today 2002.

- Improved flow control
  -is needed in long, geometrically complex shafts (enabled by advanced drilling)
  -is enabled by downhole sensors and valves
- Flow control strategy (mostly for oil recovery) involves existing as well as new control methods
  -Flow stimulation by water injection
  -Viscosity reduction by $CO_2$ injection
  -Artificial lift (surface and subsurface pumps)

Predictability of flow response to control is increasingly a limiting performance factor.

## Patterns in turbulent buoyant multiphase pipe flow

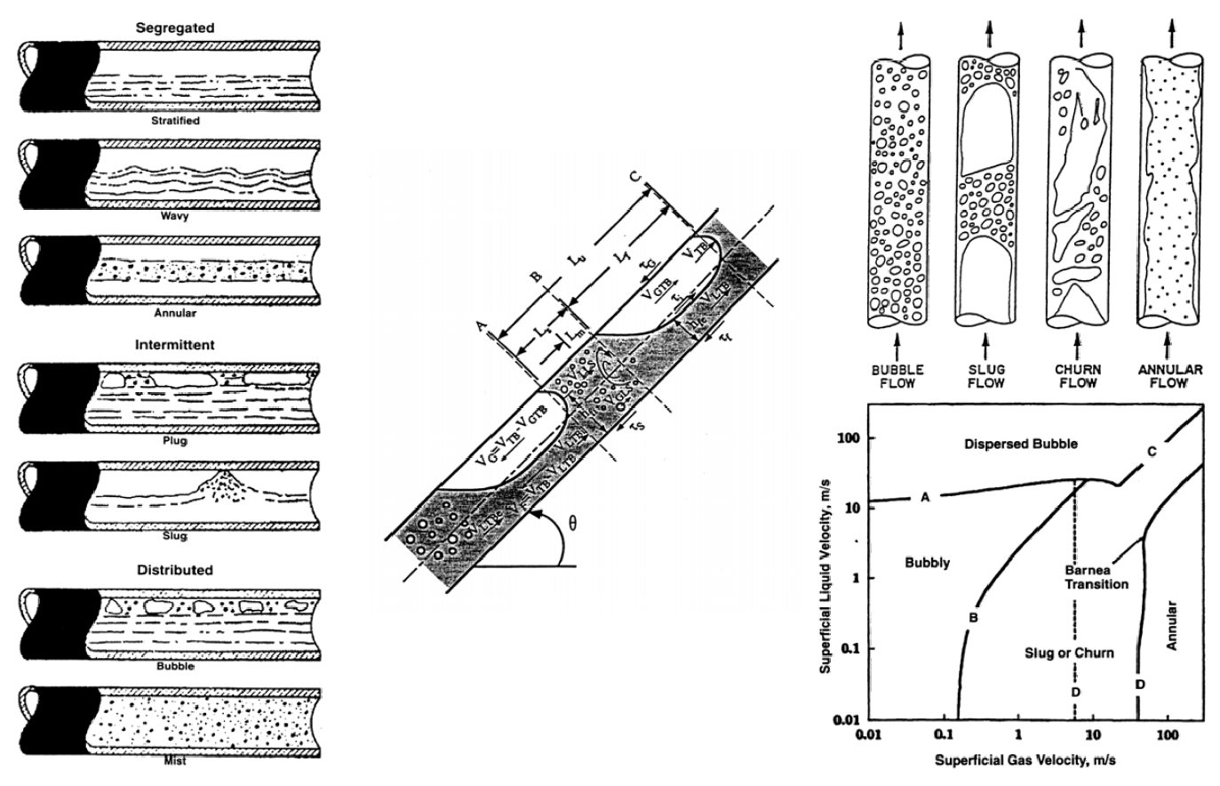


Figure taken from Physics Today 2002.

## Problem

There is currently no fundamental modeling approach that can affordably predict these patterns. Current hydraulics models involve empirical correlations based on costly tests. An adequate coverage of parameter space is unaffordable, leaving major gaps. Physics is too complicated for scale extrapolation of small scale tests. ⇒ costly large tests

## Key idea of the project

We develop and demonstrate a new fundamental flow simulation method that reliably predicts flow patterns and associated performance characteristics The technology impact is:

1. The simulation tool, benchmarked by test data, will provide a practical, affordable method for building flow databases
2. Industry can thus generate the data needed for adequate empirical representation (by engineering correlations) of wellbore hydraulics in $CO_2$ storage or oil recovery system simulations

The new tool is not the wellbore hydraulics engineering model, but an enabler of engineering models. The proposed project has broad implications:

- Addresses key CSS/gas/oil industry concerns
- Relevant to other technologies: geothermal energy, nuclear reactors (boiling heat transfer), combustion, and chemical engineering processes
- Combines ideas of stochastic turbulence models (see ODT) and mathematical tools (see level set methods) to describe (phase) interfaces

## What is the key idea in ODT models?

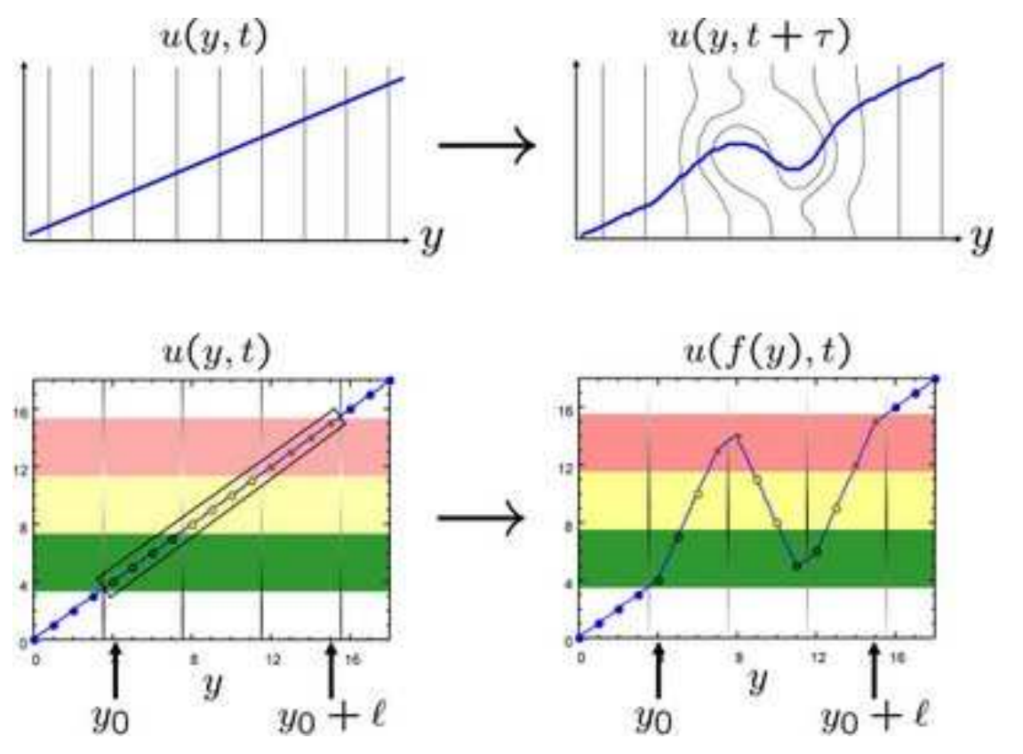
One Dimensional Turbulence (ODT), a 1D model emulating 3D turbulence, including turbulence-microphysics interactions, has been developed and extensively demonstrated during the last decade (see box to the right)

1. It combines two well-known 1D approaches:
   - The 1D boundary-layer formulation of the equations of motion, with IC's and BC's corresponding to various inhomogeneous flows: Captures the combined effects of advective and molecular transport
   - Stochastic iterated maps: capture the multi-scale dynamics of the advection-dominated (inertial) subrange of homogeneous turbulence
2. It incorporates widely used mixing-length idea

### Map-based advection

On a 1D domain, molecular evolution based on a boundary layer formulation is supplemented by an eddy process, e.g., $u_t = \nu u_{yy} +$ eddies. To specify the eddy process, we need

- the definition of an eddy (biography),
- an eddy time scale $\tau$ or frequency $f = 1/\tau$, and
- an eddy selection procedure (demography).



Effect of an eddy of size $l$ located at $z_0$ on a 1D profile.

The time, location, and length are sampled from a probability distribution based on local energetics of the turbulent field. The time scale $\tau$ can be interpreted as the turn over time of an eddy of size $l$.

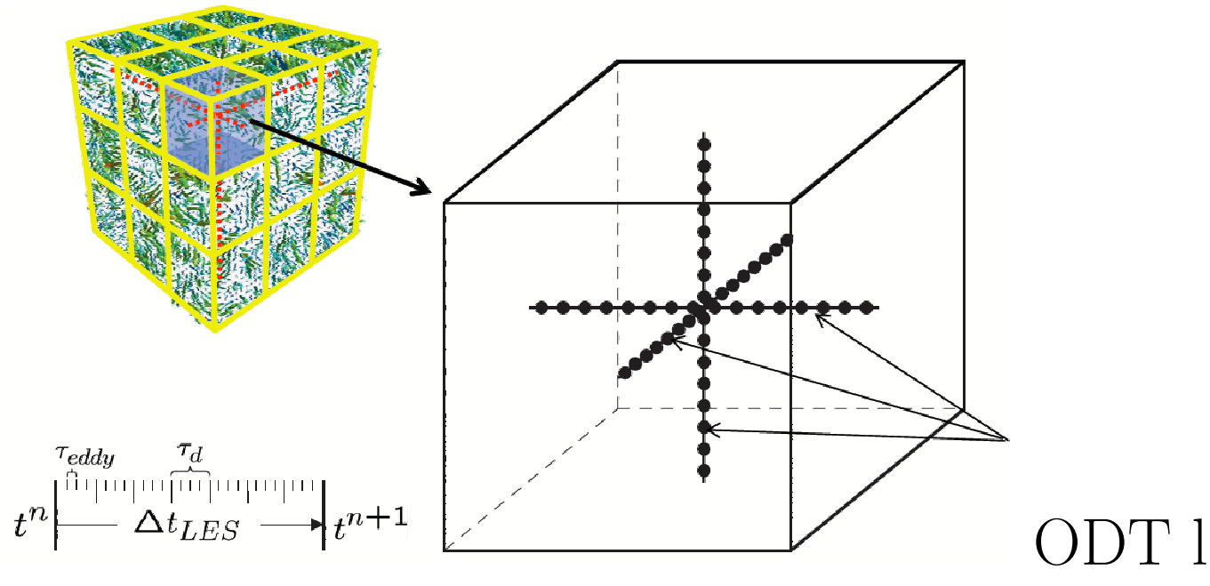
## History of ODT

ODT was initially developed as a pure 1D model, emulating 3D turbulence characteristics. The 1D domain is normally orientated in the direction of the largest scalar or velocity gradients. It has been used for pure boundary treatment in LES and later as a full subgrid scale model (ODTLES). A full 3D version called autonomous microstructure evolution (AME) taking care about fluxes on all resolved scales is the future goal. A rough overview over various applications of ODT may be found in:

1. Basic articles and ODT formulation [3, 8, 2]
2. Rayleigh-Bénard convection [16]
3. Buoyancy reversal [15]
4. Layering in stratified flows [14]
5. Nocturnal atmospheric boundary layer [7]
6. Double diffusive convection [4]
7. Combustion [1, 13, 11, 10]
8. Sub-grid closure for LES [5, 18, 9]

### Basic idea of ODTLES and AME

Compared to a resolution of a Direct Numerical Simulation (DNS) which is N cubed for N points in one direction, AME only needs O(N) points thus allowing for larger ranges in scales for a given amount of computational power. Three 1D ODT substructures are located in each LES cell in ODTLES (see figure). The three substructures are communicating with the LES and among themselves. In AME the formal split between large scales and subgrid scales (below filter scale) is no longer necessary, since ODT takes care about the entire fluxes between large scale geometry adapted flow volumes.



## Level Set Definition and Motion

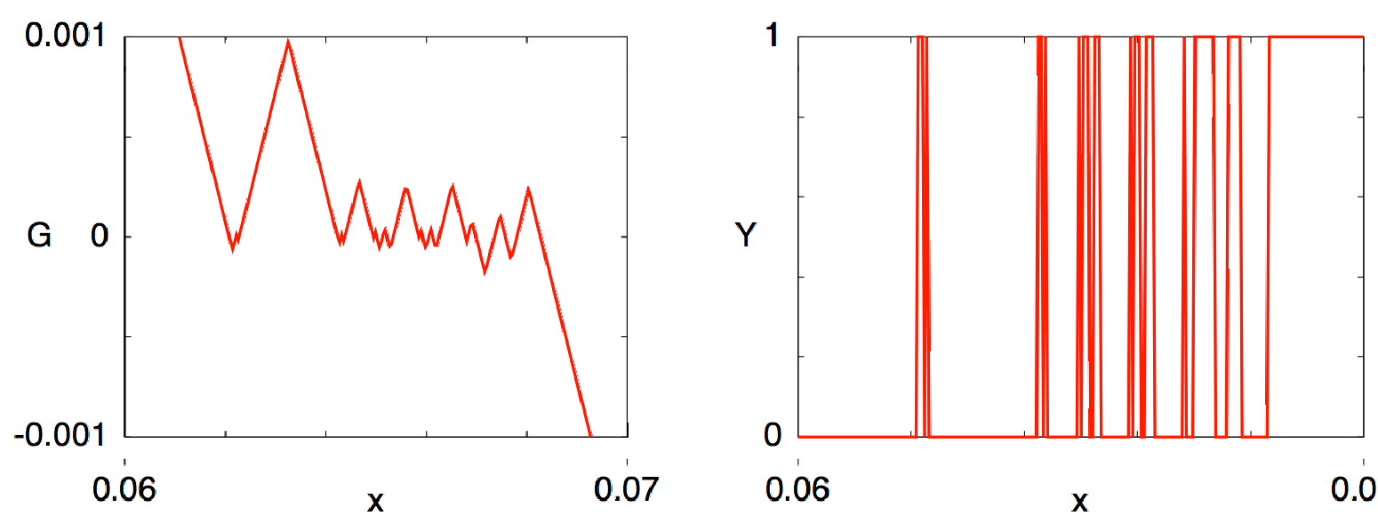
- As alternative to adaptive ODT we implicitly define the phase interface $\partial\Omega$ as $\partial\Omega = \{\boldsymbol{x} \mid \phi(\boldsymbol{x}) = 0\}$ dividing the problem into 3 subdomains:

$$\begin{aligned} \phi &> 0 \qquad \forall \boldsymbol{x} \in \Omega^+ \\ \phi &< 0 \qquad \forall \boldsymbol{x} \in \Omega^- \\ \phi &= 0 \qquad \forall \boldsymbol{x} \in \partial\Omega \end{aligned} \tag{1}$$

- Evolution of the level set function $\phi$:

$$\frac{\partial \phi}{\partial t} + (\boldsymbol{v} + s\boldsymbol{n}) \cdot \nabla\phi = 0 \tag{2}$$

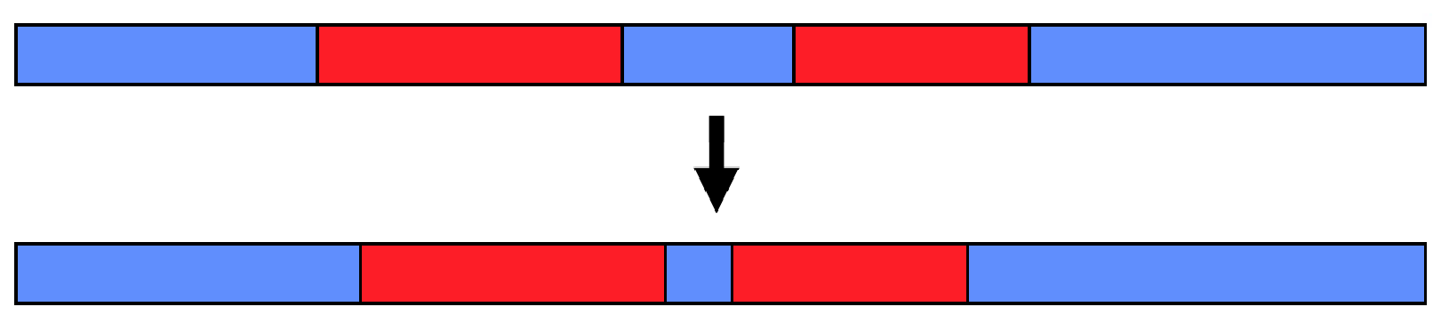
- Here the phase interval contraction rate $s$ scales dimensionally as $(2\sigma/\rho\delta)^{1/2}$ ($\sigma$ = surface tension, $\rho$ = mass density, $\delta$ = size of phase interval)
- To avoid very large or small gradients $\phi$ is initialized as a *signed distance function* ($|\nabla\phi| \equiv 1$).



Interface defined via the zero points of a levelset function (left) vs. the discontinuous picture of e.g. a mixture fraction field of one liquid component (right).

## Coupled interface/ODT motions for a physically realistic evolution

1. ODT is a line of sight through multiphase flow:
   - Sequence of phase intervals
   - Surface tension at interfaces stores pot. energy
2. ODT creates, moves, and annihilates interfaces:
   - ODT eddies create interfaces
     - Surface tension energy storage suppresses low-energy eddies
     - Resulting dynamics reflect phase-dispersion energetics
   - Interfaces move so as to reduce surface-tension energy
     - Enforces the physically prescribed rate of interface annihilation
     - Emulates phase consolidation
     - Will incorporate buoyancy and friction effects on interface motion



Interface defined via the zero points of a levelset function (left) vs. the discontinuous picture of e.g. a mixture fraction field of one liquid component (right).

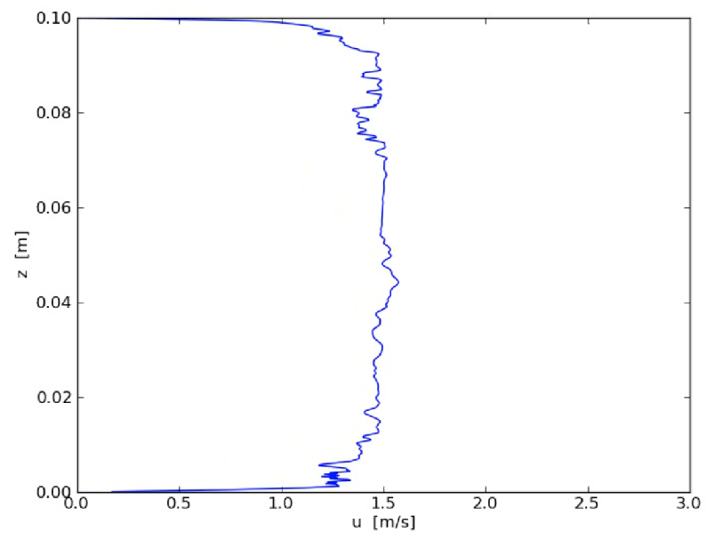
- Rate competition drives net contraction of small intervals, leading to interface annihilation, while large intervals grow
- Fluid removed from a contracting interval is transferred to second-nearest neighbors (half to each) so as to conserve both phases (red and blue)

### Surface-tension modifies the eddy time scale $\tau$

- Principle: Enforce consistency of eddies and flow (velocity and density profiles)
- Eddy: Eddy velocity ≈ $l/\tau$, so eddy energy is $\rho l^2/\tau^2$ ( $l$ = eddy size)
- Flow:
  - P = grav. pot. energy change caused by eddy
  - K = maximum kinetic energy extractable by adding wavelets to velocity components
  - A = increase of surface-tension energy due to eddy-induced phase-interface creation
  - D = energy made available by surface-tension energy release due to prior interface destruction
  - C = model constant
- Generalization of the relation determining $\tau$: $\rho\frac{l^2}{\tau^2} = C\,(K - P - A + D)$

## Work in Progress and Outlook

We start implementing the multi phase technique described before into a basic 1D ODT code. Before going to 3D pipe geometries, the comparison of our 1D model to experimental results from [20] and followers will be a first milestone. From here two ways can be followed. Parameter studies are performed with the 1D model to generate $CO_2$ data bases to develop better subgrid scale models for multiphase pipe flow which can be used in standard flow solvers. Another path is to use the 1D multiphase ODT as a building block of the above described AME formulation suitable for multiphase pipe flow simulation, and use of this formulation to attain the capability to predict various flow patterns, which appear due to the complex interaction of turbulence, buoyancy, and multiphase dynamics.



Snapshot of the stream-wise velocity field in an ODT channel flow simulation driven by a constant pressure gradient.

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