"Toward Engineering Simulation in the Petrochemical Industry: From Discovery to End-Use"

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Observation

• Innovation and engineering drive many of future technologies in energy production, processing, and end use.

• Recent years has shown a broad application and accelerating rate of adoption of engineering Simulation tools
  – Coupling of reservoir and well bore
  – Drilling and production
  – Storage and Transport
  – Refining and processing
  – End use design for example:
    • Formulation and engine performance
  – Material handling and processing
    • Extrusion
    • blow molding

• The rapid growth and a broader acceptance are due:
  – Advanced computational and numerical techniques,
  – Enhanced physical models
  – Usability improvements,
Objectives

- Brief overview of ANSYS activities in Petrochemical
  - Review the breath of the engineering simulation applications
  - Provide an update on some of the underlying technologies
    - Meshing
    - FSI
    - Particulate flows
    - In-cylinder-combustion
    - Parallel processing
  - Provide examples of work underway at ANSYS for Advanced Petrochemical applications
  - Flow assurance
    - Slug flow
    - Sand and water management
Sample examples Drilling/Production
Sample examples Refining/Processing
Offshore Hydrodynamics

- Wave impact
- Sloshing
- Transport

• Offshore Structures
  - Fixed
    - Steel Jackets
    - Concrete
  - Floating
    - FPSOs
    - SPARS
    - Semi-Submersibles
  - Risers
  - Ship
    - Design
    - Offloading
    - Shielding
  - Applications
    - Mooring systems
    - Lifting operation – AMOG
    - jacket launch

Transportation of Spar Truss on Heavy Lift Vessel
Petrochemical Industry Advanced Technology Needs

- **Selected list:**
  - Complex geometry and grid motion
  - Wide range of numerics
  - Advanced physics
    - Combustion and Reaction
    - Multiphase
    - Turbulence-Chemistry
  - Multi-scale
  - Multiphysics
  - HPC and Parallel computing
Recent Software Development Activities

- **Meshing**
  - Wrapping Technology
  - Immersed boundary condition
- **Multiphase**
- **In-Cylinder Combustion**
- **Parallel processing**
Wrapping Technology
- Clean up complex geometry
- Accelerate meshing

Immersed boundary condition
- Simulations @ non-body conforming meshes
- Reduced time for geometry & mesh preparation
- Boundary conditions via reconstruction schemes
- **Mesh morphing**
  - Cylindrical component displacement option
  - Mesh quality histogram in ‘out’ file
- **One-way and two way coupling**
- **Surface loads**
  - Forces
  - Energy fluxes
- **Volume loads**
  - Temperature
• Setup of multiple configurations
• Re-meshing
• Combustion
• Particle tracking & sprays
• Wall films
• ...
Multi-Phase – Euler-Lagrange

- Spray break-up models
  - Primary – Huh & Gosman
  - Secondary

- Validation report
  - Collaboration with Robert Bosch

Hiroyasu & Kadota, case 1

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CFX - Multi-Phase – Euler-Lagrange
Multi-Phase, Multi-fluid VOF

- Multi-fluid free surface flow model (VoF)
  - Separate velocities for each phase
  - Explicit interface tracking scheme
- Multi-fluid free surface flow model (VoF)
  - Heterogeneous model
  - Separate velocities for each phase
  - Explicit interface tracking scheme
Modeling particulate systems

- Sedimentation, transport
- Separators & reactors
- Spray dryer and congealers
- Coaters and granulators
- Filtration products
- Slurry flows
- Solid suspension
- Trickle bed reactors
- Risers
- Fluidized beds
- Pneumatic conveyors,
- hoppers, silos
- ...
Diluted vs. Dense Flow

- **1-way coupling**: negligible effect on turbulence
- **2-way coupling**: particles enhance turbulence
- **4-way coupling**: particles reduce turbulence

**Relative motion between particles**
- Dilute: Large
- Dense: Small

**Particle-particle interaction**
- Dilute: Weak
- Dense: Strong

**Apparent viscosity of the solid phase**
- Dilute: Particle-fluid interactions
- Dense: Particle-particle interaction
Overview of Modeling Approaches

- Direct Numerical Simulation
  - Trajectories of individual particles
  - Flow around individual particles

- Eulerian Granular
  - Continuum model (multi-dimension)
  - Local averaging

- Particle Motion
  - Euler-Lagrangian
  - Grid elements

- Fluid Motion
  - DNS/DEM/MPM

Concept illustration borrowed from Prof. Tsuji Presentation at WCPT5, April 2006
Particle Models Available

- Modeling particulate flows have been an area of focus for over a decade; current capabilities include:
  - Particle Methods
    - DPM for dilute phase (steady and time dependent)
    - Macroscopic Particle Model (MPM) for large particles
    - Dense-phase discrete particle model (DP-DPM) for dense flows with large size distributions
  - Continuous Methods
    - Euler-Granular
    - Euler-Granular with Frictional viscosity for dense phase
  - Hybrid Methods
    - Coupled simulations
    - DEM
<table>
<thead>
<tr>
<th>Method</th>
<th>Particle to particle interactions</th>
<th>Coupling with cont. phase</th>
<th>Additional physics &amp; chemistry</th>
<th>Particle shape, size distribution</th>
<th>Order of # of particles</th>
<th>Computation speed &amp; parallelization</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEM</td>
<td>Direct contact and other forces implementation</td>
<td>None or through ext. CFD code</td>
<td>Not implemented</td>
<td>Arbitrary (clustered spheres) shape &amp; distribution</td>
<td>~10^5</td>
<td>Strongly dependent on # of particles, not parallelized, Rel. slow</td>
</tr>
<tr>
<td>DPM</td>
<td>Collisions &amp; breakup indirectly; packing limit not accounted</td>
<td>Correlation-based drag force</td>
<td>Coupled with all std. Fluent models, easy to customize</td>
<td>Spherical and ellipsoidal</td>
<td>~10^6</td>
<td>Very fast, parallelized</td>
</tr>
<tr>
<td>DP-DPM</td>
<td>Particles are represented by clusters, packing limit is maintained</td>
<td>Correlation-based drag force</td>
<td>Coupled with all std. Fluent models, easy to customize</td>
<td>Spherical, arbitrary size distribution available</td>
<td>No limit on part/clusters (tested up to ~ 2.5x10^5)</td>
<td>Rel. fast, affected by mesh size &amp; # of particles, parallelized</td>
</tr>
<tr>
<td>MPM</td>
<td>Direct contact and other forces implementation</td>
<td>Drag &amp; torque resolved</td>
<td>Further customization possible</td>
<td>Spherical*, arbitrary distribution</td>
<td>~10^5</td>
<td>Slow, parallel tracking (interactions not parallel)</td>
</tr>
<tr>
<td>Euler Granular</td>
<td>Indirect: solid pressure &amp; radial distr., other forces implemented indirectly</td>
<td>Cell-avg. drag, lift &amp; other inter-ph. terms</td>
<td>Coupled with all std. Fluent models; easier to customize</td>
<td>Spherical; Size dist. through population balance</td>
<td>Practically unlimited</td>
<td>Fast, depends on the mesh size &amp; physics only, parallelized</td>
</tr>
</tbody>
</table>

*arbitrary shapes being tested

!!! This table is for tentative and qualitative comparison
!!! Because of a continuous development, models continue to evolve
Challenge Problem: gas-solid Riser

- Expect risers to be a tough challenge
  - Complex multi-scale physics
  - Strands, clusters etc.
  - May stretch validity of assumptions of parcels
- Preliminary results show some promise shown here
- More qualitative validation is needed
**ANSYS Technology Update**

**Parallel Computing**

- **Discretization & Solution**
  - Optimization of equation assembly & solution
  - Iteratively bounded advection & transient scheme for turbulence quantities

- **Much larger problems are being molded**

- **Scalability, especially on large clusters**
  - Example; Opteron/EM64T Inamd64 version
  - Currently under testing
    - 1 billion cell case
    - 700 million cells per processor per core
    - Opteron/EM64T Inamd64
Advanced oil and gas applications

• Flow Assurance
• **Motivation**
  – The trends in deep and ultradeep production requires robust understanding and planning of:
    • Production Enhancement
    • Flow Assurance in increasingly demanding conditions
  – Flow Assurance requires a systematic analysis including
    • thermal and hydraulic performance
    • multi-phase flow
      – Slugging
      – Water and Sand management
  – hydrates and paraffin or wax precipitation
Produced water

- Produced water is not a product
- For offshore operations, the disposal
  - Re-injection to the formation
  - Transport onshore.
- Produced water is “contaminated” with high salinity, oil and metal
- Polishing produced water
  - clarifiers,
  - hydrocyclones,
  - membrane separation,
  - ultraviolet light treatment,
  - various separators
- Engineering Simulations tools are used to
  - Reduce risk
  - Increase reliability of equipment and processes.
Application Focus
Sand Management and Transport

• Sand is often produced out of the reservoir in both onshore and offshore production systems, particularly in reservoirs that have a low formation strength.

• Sand production may be continuous, or sudden - as when a gravel pack fails.

• The sediment consists of finely divided solids that may be drilling mud or sand or scale picked up during the transport of the oil.

• Sand deposition could lead to corrosion of the pipeline.

• Problem of sand deposition and re-entrainment
  – Inclined pipelines, pigging sand plug pipeline.
Slurry Flow Regimes

- Slurry flow is classified into different regimes
- The transition between regimes depends on
  - Solids concentration
  - Velocity
  - Particle Diameter
  - Turbulence
- Mostly derived for high sand concentrations (>1%) and large particle diameter (>100um)
- Typical:
  - 5-50 lb sand / 1000 bbl liquid
  - $U_{SL}/U_{SS} \sim 50000-500000^{**}$


Study Objectives

• Lack of data on low volume fraction \(<1\text{vol}\%\) and small diameter \(<50\mu\text{m}\)

• Validation work using experimental data
  – Range of volume fractions
  – Range of sand particle diameter
  – Different pipeline diameters

• Gain confidence in modeling methodology and extend approach to:
  – Low concentrations and particle diameter
  – Pipeline orientation

• Influence of turbulent fluctuations
  – Interphase turbulent momentum transfer
    • Drift velocity
  – Volume fraction diffusion
Pressure Drop Validation

• Experimental data from:

• Experimental Conditions
  – Horizontally straight pipeline length, $L = 1.4$ m
  – Pipe I.D. = 0.0221 m
  – Silica sand–water slurry
    • Water density $\rho = 998.2 \text{ kg/m}^3$
    • Sand density $\rho = 2381 \text{ kg/m}^3$
    • Sand diameter $d_p = 0.000097–0.00011 \text{ m}$
  – Inlet sand concentration = 20 vol%

• Assumed fully developed, fully mixed inlet slurry flow

• Mesh size: 140K cells
Pressure Drop Validation

- Good agreement with experimental data
- The influence of the solids volume fraction is captured with the Wen & Yu drag model
- Flow regime – heterogeneous transport
Predicting Solids Dispersion

• Analysis of the following variables:
  – Slurry velocity
  – Solids concentration
  – Solid particle diameter
  – Mesh: 0.5 million cells

<table>
<thead>
<tr>
<th></th>
<th>34</th>
<th>27</th>
<th>27</th>
<th>34</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solids conc., vol%</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Particle dia. (d_p) (µm)</td>
<td>120</td>
<td>120</td>
<td>120</td>
<td>370</td>
</tr>
<tr>
<td>Velocity (m/s)</td>
<td>6.00 0</td>
<td>6.000</td>
<td>2.000</td>
<td>6.000</td>
</tr>
</tbody>
</table>


Well-mixed Slurry (Sand/Water) 150 mm diameter pipe \(\rho_{\text{sand}}=2650\ \text{kg/m}^3\) 3 m

Test section

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Influence of Particle Concentration

- Flow regime is nearly homogeneous
  - $V >> V_{\text{critical}}$
- Solids almost uniformly distributed across the pipe diameter
- Experimental measurements mostly in the center of the pipe
  - Good agreement with simulation results
- Drop in slurry concentration near pipe wall

$V_{\text{slurry}} = 6 \text{ m/s}$
$\rho_p = 120 \mu\text{m}$
Influence of Particle Diameter

- Flow regime is heterogeneous transport
  - \( V >> V_{\text{critical}} \)
- Solids concentration increases near the pipe bottom with the increase in particle diameter
- Experimental measurements in good agreement with simulation results
- Drop in slurry concentration near pipe wall
Influence of Slurry Velocity

- Flow regime is heterogeneous transport
  - $V > V_{\text{critical}}$
- Solids concentration profile changes with drop in velocity
- Increase in slurry concentration near pipe wall at lower velocity
- As the granular temperature increases, particles are pushed from the wall
- Dissipation from collision is insufficient to counteract the higher values

$d_p = 120 \, \mu m$

$Y / D$

Solids Volume Fraction

Fluent CFD: $V_s = 2 \, m/s, C_s = 27\%$
Fluent CFD: $V_s = 6 \, m/s, C_s = 27\%$
Fluent CFD: $V_s = 2 \, m/s, C_s = 34\%$
Fluent CFD: $V_s = 6 \, m/s, C_s = 34\%$
Matousek, 2002 ($V_s = 6 \, m/s, C_s = 34\%$)
• Eulerian granular multiphase was applied to model dilute and dense slurry flows in pipes
• Good agreement was obtained for the pressure gradient and the solids distribution
• The influence of turbulence on the interphase momentum exchange (Eulerian) is required for this class of problems
• For dilute flows, incorporating the influence of turbulent dispersion in the volume fraction equation maybe required
• Further studies - pipe orientation, re-entrainment, flow regime with stationary bed, polydispersed solids
Application Focus
Predicting Slug Flow

• Multiphase pipeline analysis for flow assurance
  – Hydrodynamic slugging
  – Terrain slugging

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Hydrodynamic slugging
Experimental Setup

• Experiments conducted in WASP at Imperial College
  – No influence of downstream conditions on upstream gas/liquid flow rates
• 78 mm diameter x 37 m pipe
• 0.5 m long inlet section with separate gas/liquid inlets and splitter plate
• Air/Water system
  – $v_{SG} = 4.64$ m/s
  – $v_{SL} = 0.61$ m/s
  – Inlet pressure = 1.15 bar
• Expected flow regime is slug flow
Hydrodynamic slugging
Numerical Setup

• **Numerics**
  – NITA with Fractional step
  – Default Solver Controls
  – PRESTO! and First-order discretization
  – Green gauss cell-based gradient solver
  – Realizable k-epsilon
  – Geo-reconstruct

• **Phase Interaction**
  – Surface tension = 0.072 N/m

• **Calculation time on HPC queue (Opteron/IB)**
  – Global Courant Number = 1
  – Variable time step ~ 1e-5 – 1e-4s
  – Solution time = 6 s / iteration – 265475 iterations/87.09 seconds real time on 16 CPUs
  – Solution time = ~80 hours of CPU time per second of real flow time

• **Mesh Size 1.03 Million**
Hydrodynamic Slugging with VOF

Interface height at 53.23 s

Snapshot of interface at 53.23 s
Comparison of Height Profiles

- Characteristic gradual rise in interface height followed by rapid drop is reproduced by the VOF model.
- Lower dips towards the end of the pipe reproduced.
- Stratified-wavy interface near inlet is reproduced.

VOF

Area-Weighted Average Y-Coordinate

L.W.Avg Y-Coord
- z=1.5
- z=13.90
- z=34.5

Convergence history of Y-Coordinate

Convergence history of Y-Coordinate

Δt_{slug passage} ~ 5 seconds

Top of pipe

Experimental

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• Experimentally determined slug frequency varies along length of pipe though slugs formed by ~5m remain relatively intact to the end of the pipe
  – Slug frequency ~ 0.2 – 0.3 s\(^{-1}\)
  – Range of time interval between slugs of 1 – 10 seconds
• The VOF simulation shows similar range of slug interval and frequency
Recap

- Engineering Simulation tools are being used to solve a broad range of applications in the petrochemical and related industries.
- A selected set of related software development capabilities we reviewed. Highlighting, meshing, FSI, multiphase, and parallel processing.
- A review of application of CFD to predicating slugs and sand transport was presented.
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