SRS 2H Evaporator Transport Modeling

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9 January 2001

RELEVANCE

- Provide insight on the temperature distribution and flow in the evaporator
- Integrate results of concurrent studies on formation of aluminosilicate deposits
- Provide a framework and reference for more advanced transport modeling

GOALS

- Construct and analyze a tractable model of flow and temperature by the end of February 2001

- Produce technical report on 22 March 2001

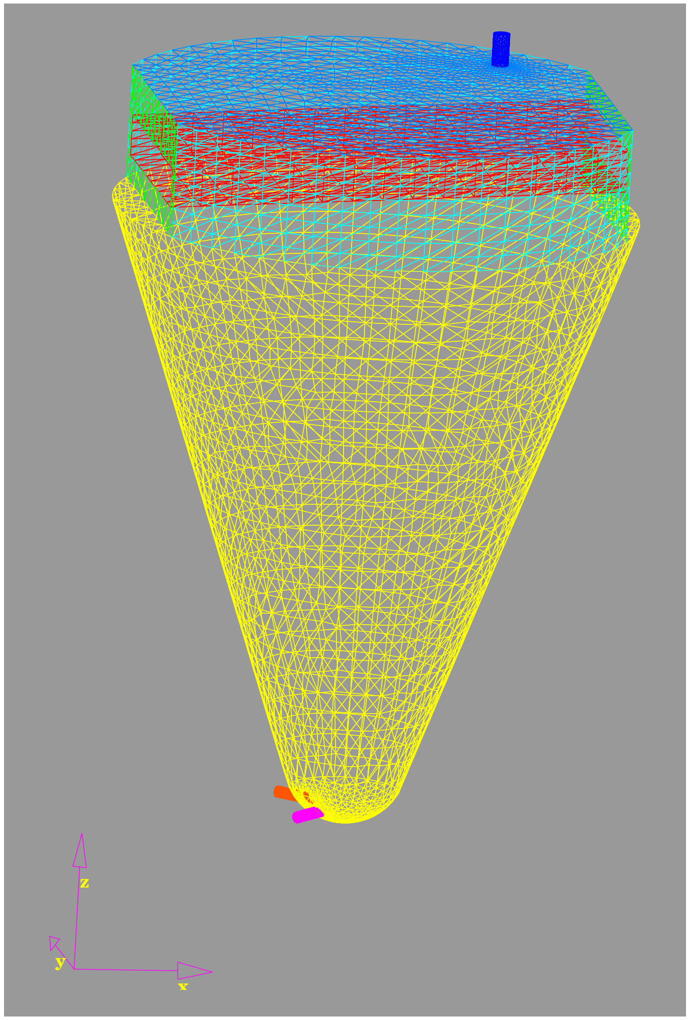
OUTLINE

- Geometric model
- Equations of transport & parameters (dimensionless groups)
- Boundary conditions
- Parametric studies and results
- Solution method & algorithms
- Outlook

GEOMETRIC MODEL

- Three-dimensional
- Based on actual dimensions (tech. drawings & system design description doc.)
- Components included
  1. Artificial shear-free liquid interface
  2. Feed tube
  3. Tube bundle envelope
  4. Cylindric-conical vessel
  5. Discharge lift
  6. Lower lance
- Major items neglected
  - Entire overhead system
  - Warming coil and auxiliaries
  - All other pipes/tubes
  - Internal stay rods and structural beams

GEOMETRIC MODEL



EAST-WEST VERTICAL CROSS SECTION (DWG No. D-10578)

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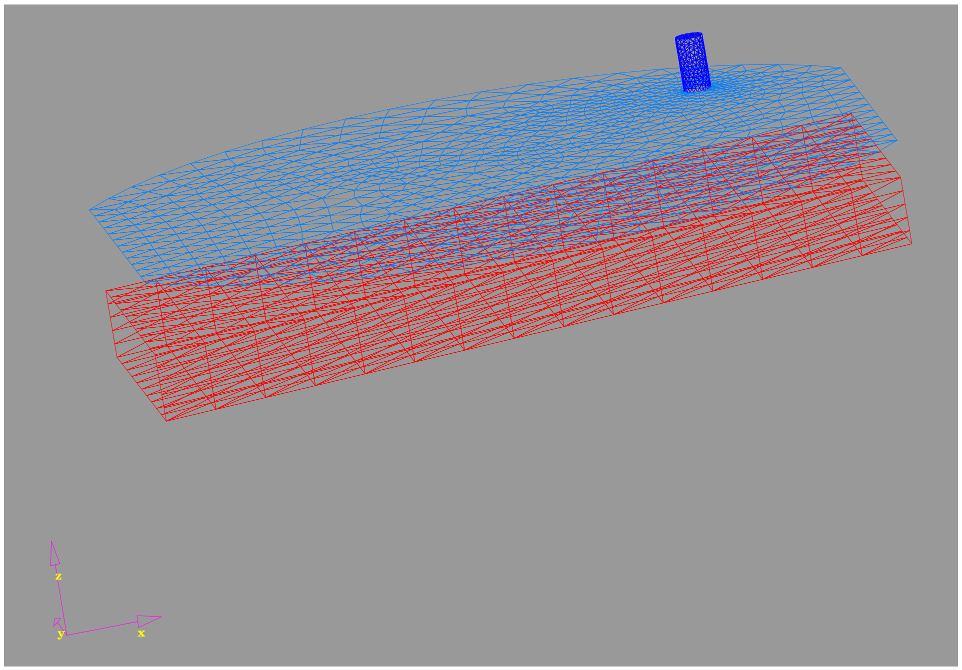
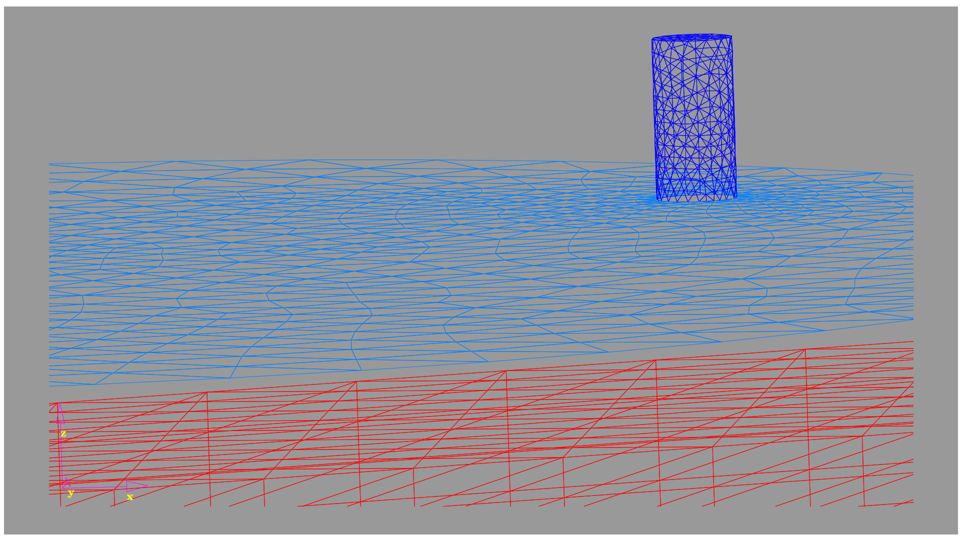
ARTIFICIAL SHEAR-FREE LIQUID INTERFACE



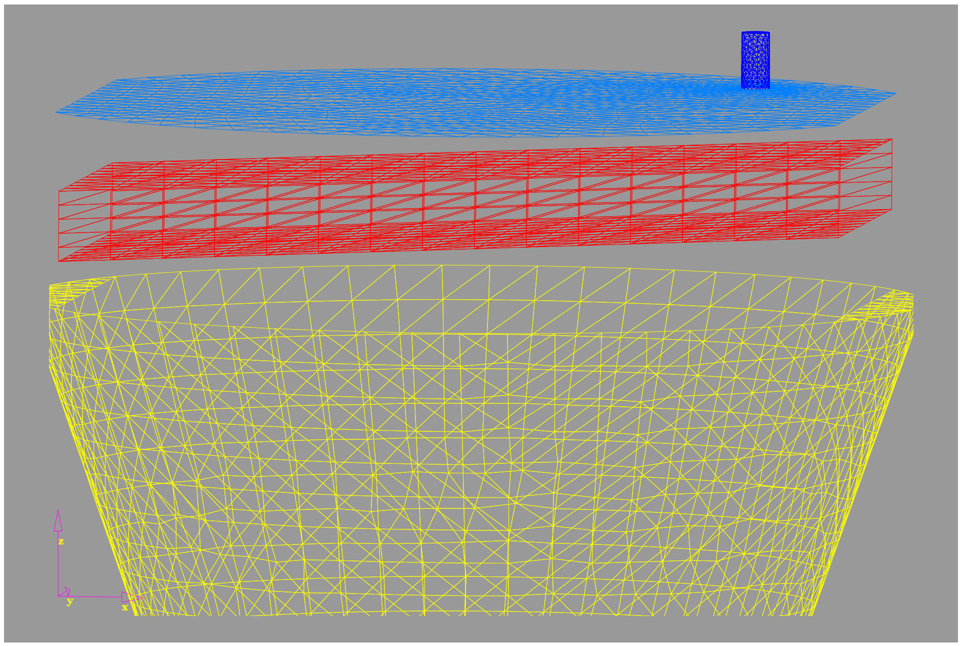
- Upper boundary of the model
- Flat, positioned 6" above the inlet of the tube bundle (East side)
- Intersected perpendicularly by the feed tube (North-East)

FEED TUBE



- 3"-diameter submerged into the liquid (not implemented yet)
- Positioned at the North-East side (B nozzle, 57°)
- Discharge cross section cut at an angle
- Needs additional information (length, orientation of discharge section)
- Needs careful attention to thermal entry length (see B.C.)

TUBE BUNDLE ENVELOPE



- Duct of rectangular cross section wrapping the tube bundle (240 tubes)
- Traverses the evaporator from East (steam inlet) to West (steam outlet)
- 3.4-ft wide; 7-ft long; 0.625-ft deep;
- Neglects cross flow through bundle
- Individual tubes are 0.758"-diameter; 0.5" gap

TUBE BUNDLE—EAST-WEST VERTICAL CROSS SECTION

(DWG No. D-10760)

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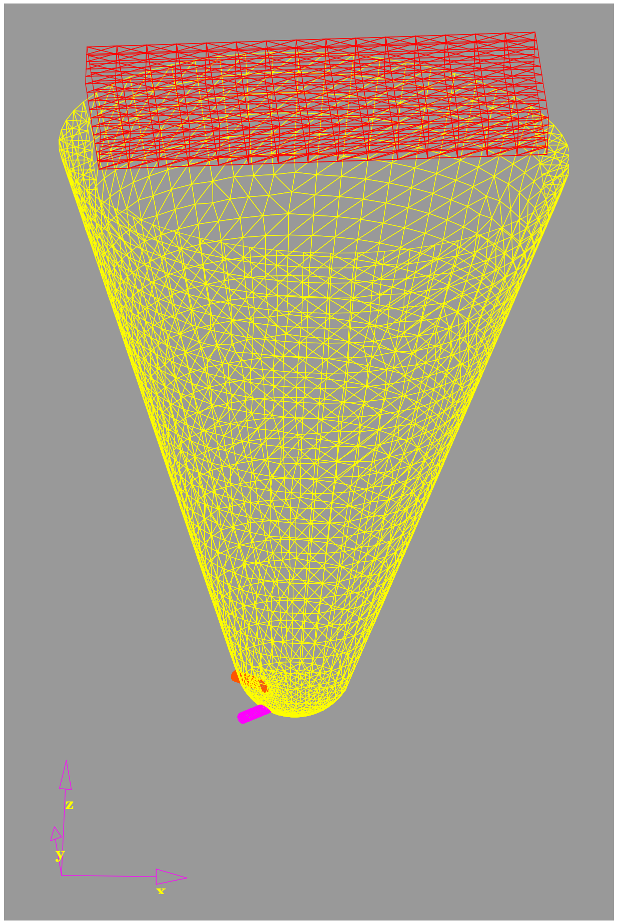
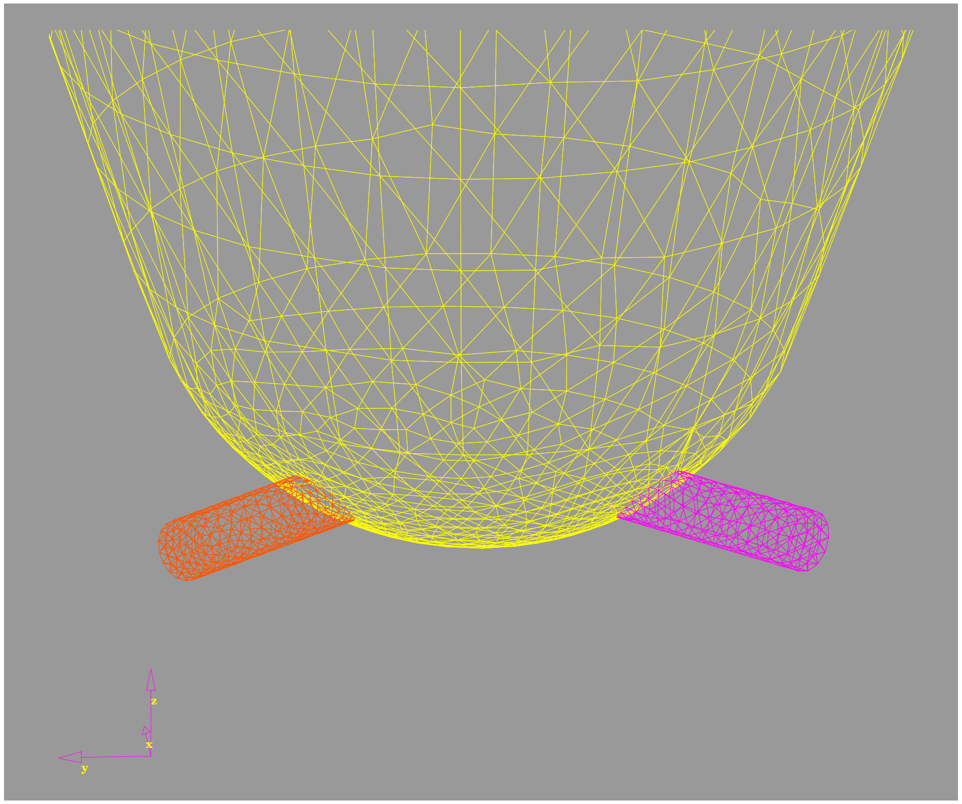
CYLINDRIC-CONICAL VESSEL



- Cylindric section housing the bundle envelope; 4-ft diameter; 1.75-ft long
- Lower conical section 9-ft long with smallest diameter of 0.84 ft
- Spherical cap 0.5-ft deep at the bottom
- Spherical cap is intersected by the lower lance and discharge lift

DISCHARGE LIFT



- South-West positioning (45°)
- Intersects the spherical cap horizontally 3" from the bottom
- 2"-diameter pipe
- Two discharge lifts shown; only the South-West will be used

DISCHARGE LIFT Q (DWG No. D-10763)

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DISCHARGE LIFT Q—TOP VIEW (DWG No. D-10763)

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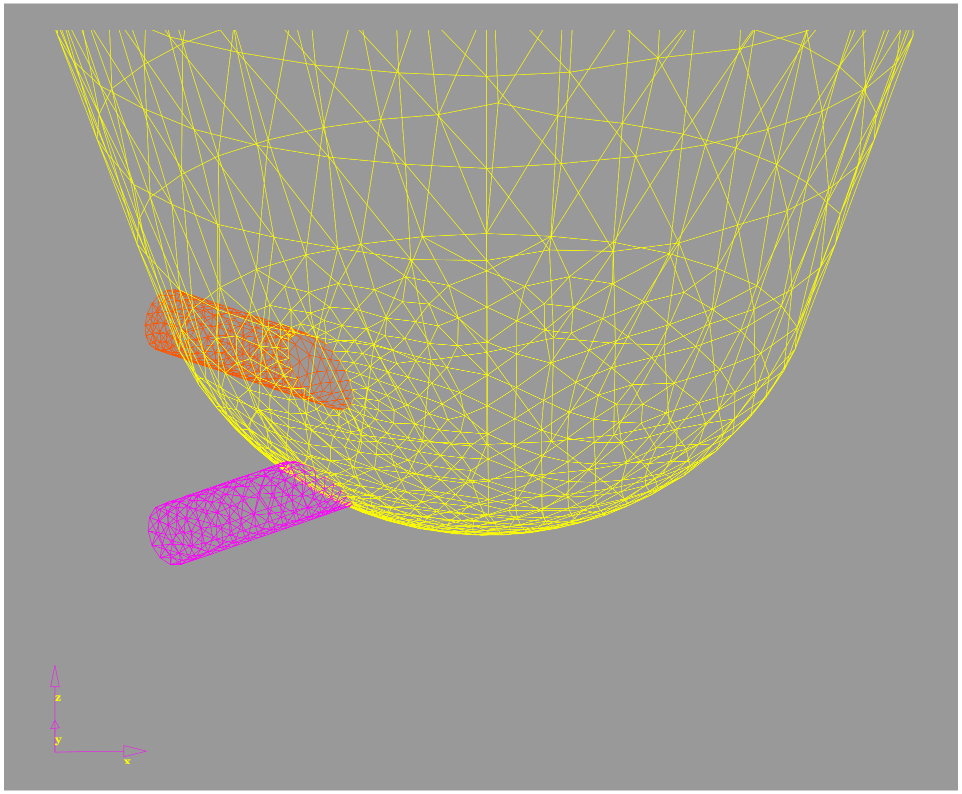
LOWER LANCE



- Positioned South pointing North
- Intersects the spherical cap horizontally 3" from the bottom
- 1.5"-diameter pipe
- Not implemented yet

EQUATIONS OF TRANSPORT (FLOW & HEAT)

$$\mathrm{div}_{\boldsymbol{x}}(\boldsymbol{v} \otimes \boldsymbol{v}) = \mathrm{div}_{\boldsymbol{x}}\, \boldsymbol{T} - Gr\,\theta \boldsymbol{g} \qquad \forall\ \boldsymbol{x} \in \Omega,$$

$$\mathrm{div}_{\boldsymbol{x}}\, \boldsymbol{v} = 0 \qquad \forall\ \boldsymbol{x} \in \Omega,$$

$$Pr\,\mathrm{div}_{\boldsymbol{x}}(\theta \boldsymbol{v}) = \mathrm{div}_{\boldsymbol{x}}(\nabla\,\theta) \qquad \forall\ \boldsymbol{x} \in \Omega,$$

with constitutive equation of stress

$$\boldsymbol{T}(\boldsymbol{x}) := -p(\boldsymbol{x})\boldsymbol{I} + \nabla_{\boldsymbol{x}}\, \boldsymbol{v} + \nabla_{\boldsymbol{x}}\, \boldsymbol{v}^{\mathsf{T}} \qquad \forall\ \boldsymbol{x} \in \Omega.$$

- 3-D, laminar, steady-state flow of a Newtonian incompressible fluid
- Boussinesq buoyancy term coupling bulk fluid flow and heat transport
- Fields: velocity $\boldsymbol{v}$, pressure p, and temperature θ

AVERAGE PHYSICAL PROPERTIES OF SIMULANT			
ρ	mass density	1.25	$\mathrm{kg\,m^{-3}}$
μ	dynamic viscosity	$2.54\,10^{-3}$	$\mathrm{kg\,m^{-1}\,s^{-1}}$
β	thermal expansion coef.	$5.5\,10^{-4}$	$\mathrm{K^{-1}}$
C_p	heat capacity	$3.7\,10^{3}$	$\mathrm{J\,kg^{-3}\,K^{-1}}$
κ	thermal conductivity	$6.8\,10^{-1}$	$\mathrm{W\,m^{-1}\,K^{-1}}$

From Bostick and Steele, Thermal and Physical Property Determinations for SRS Waste Simulant Solutions, ORNL/TM-1999/133

FIELDS		UNIT
$\boldsymbol{v}$	velocity	$\frac{\mu}{\rho\,D}$
p	pressure	$\frac{\mu^2}{\rho\,D^2}$
Θ	ref. temperature difference	$T_h - T_f$ $(\Theta = \frac{T-T_f}{T_h-T_f})$

PARAMETERS & CONSTANTS			
T_f	feed temperature	$323–363$ $(50–90)$	(°K)(°C)
T_h	tube bundle temp.	$443–463$ $(170–190)$	(°K) (°C)
T_l	lance temperature	$443–463$ $(170–190)$	(°K) (°C)
g	gravity	9.81	$\mathrm{m\,s^{-2}}$
D	ref. diameter	2.4 (8)	m (ft)
$\mathcal{Q}_f$	feed flow rate	$1.6\,10^{-3}$ (25)	$\mathrm{m^3\,s^{-1}}$ (gpm)
$\mathcal{Q}_d$	discharge lift	$6.4\,10^{-3}$ (10)	$\mathrm{m^3\,s^{-1}}$ (gpm)
$\mathcal{Q}_l$	lance flow rate	? (?)	$\mathrm{m^3\,s^{-1}}$ (gpm)

DIMENSIONLESS GROUPS		SIGNIFICANCE	RANGE
$Gr := \frac{\rho^2\, g\, D^3\, \beta\, (T_h - T_f)}{\mu^2}$	Grashof	$\frac{\text{buoyance force}}{\text{viscous force}}$	$2.7–1.5\,10^6$
$Pr := \frac{C_p\, \mu}{\kappa}$	Prandtl	$\frac{\text{viscous diffusion}}{\text{heat diffusion}}$	14

- Relatively small Grashof number

BOUNDARY CONDITIONS

- Artificial shear-free liquid interface (surface $\mathscr{S}_1$)
  - Null traction: $\boxed{\boldsymbol{T}\boldsymbol{n} = \boldsymbol{0} \quad \text{on} \quad \mathscr{S}_1}$ $\quad \boldsymbol{n} \perp \mathscr{S}_1$
    - This condition allows flow through the interface
  - No diffusive heat flux: $\boxed{\partial_{\boldsymbol{n}}\Theta = 0 \quad \text{on} \quad \mathscr{S}_1}$
    - Heat is removed at the interface by convection

- Feed tube (tube wall $\mathscr{S}_2$)
  - No slip condition: $\boxed{\boldsymbol{v} = \boldsymbol{0} \quad \text{on} \quad \mathscr{S}_2}$
  - Constant feed temperature: $\boxed{\Theta = 0 \quad \text{on} \quad \mathscr{S}_2}$

- Feed tube (discharge $\mathscr{S}_3$)
  - Specified feed flow rate: $\boxed{\boldsymbol{v} = -Re_f\, \boldsymbol{i}_z \quad \text{on} \quad \mathscr{S}_3}$
  - Constant feed temperature: $\boxed{\Theta = 0 \quad \text{on} \quad \mathscr{S}_3}$
  - Feed tube Reynolds number $Re_f = \frac{4\,\rho_f\,\mathscr{Q}_f}{\pi\,d\,\mu_f} = 13$
  - Peclet number $Pe = Re\,\mathrm{Pr} = 182$
  - Thermal entry length $\approx Pe\,d/\lambda = 4\,\mathrm{m} \approx 12\,\mathrm{ft}$

- Tube bundle envelope ($\mathscr{S}_4$)
  - No slip condition: $\boxed{\boldsymbol{v} = \boldsymbol{0} \quad \text{on} \quad \mathscr{S}_4}$
  - Constant temperature: $\boxed{\Theta = 1 \quad \text{on} \quad \mathscr{S}_4}$

- Cylindric-conical vessel (discharge $\mathscr{S}_5$)
  - No slip condition: $\boxed{\boldsymbol{v} = \boldsymbol{0} \quad \text{on} \quad \mathscr{S}_5}$
  - Insulated: $\boxed{\partial_{\boldsymbol{n}}\Theta = 0 \quad \text{on} \quad \mathscr{S}_5}$
- Discharge lift (tube wall $\mathscr{S}_6$ and discharge outlet $\mathscr{S}_7$)
  - No slip condition: $\boxed{\boldsymbol{v} = \boldsymbol{0} \quad \text{on} \quad \mathscr{S}_6}$
  - Insulated: $\boxed{\partial_{\boldsymbol{n}}\Theta = 0 \quad \text{on} \quad \mathscr{S}_6}$
  - Specified feed flow rate: $\boxed{\boldsymbol{v} = Re_d\, \boldsymbol{i}_r \quad \text{on} \quad \mathscr{S}_7}$
    * Discharge Reynolds number $Re_d = \frac{4\,\rho_d\,\mathscr{Q}_d}{\pi\, d\,\mu_d} = 3.5$ (assuming 1.4 specific gravity)
  - Fully developed $\boxed{\partial_{\boldsymbol{n}}\Theta = 0 \quad \text{on} \quad \mathscr{S}_7}$

- Lance ($\mathscr{S}_8$)
  - Specified flow rate: $\boxed{\boldsymbol{v} = -Re_l\,\boldsymbol{i}_y \quad \text{on} \quad \mathscr{S}_8}$
    - Lance Reynolds number $Re_l = \frac{4\,\rho_l\,\mathscr{Q}_l}{\pi\,d\,\mu_l} = ?$
  - Specified temperature $\boxed{\Theta = 1 \quad \text{on} \quad \mathscr{S}_8}$

$\longrightarrow$ Boundary conditions add three Reynolds number: Re_f, Re_d, Re_l (the first two are small)

PARAMETRIC STUDIES & RESULTS

- Compute velocity, temperature and pressure fields for 3 sets of values of five parameters: Gr, Pr, Re_f, Re_d, Re_l
- Visualize the temperature and speed of the flow pointwise
- Visualize trajectories of fluid particles released at the feed and their temperature history

SOLUTION METHOD AND ALGORITHMS

$$
\begin{aligned}
Re\ \nabla_{\boldsymbol{x}} \boldsymbol{v}\, \boldsymbol{v}(\boldsymbol{x}) &= \mathrm{div}_{\boldsymbol{x}} \boldsymbol{T} & \forall\ \boldsymbol{x} \in \Omega\ , \\
\mathrm{div}_{\boldsymbol{x}} \boldsymbol{v} &= 0 & \forall\ \boldsymbol{x} \in \Omega\ , \\
\boldsymbol{v}(\boldsymbol{x}) &= \boldsymbol{v}_b(\boldsymbol{x}) & \forall\ \boldsymbol{x} \in \partial\Omega\,.
\end{aligned}
$$

$\boldsymbol{T}(\boldsymbol{x}) := -p(\boldsymbol{x})\boldsymbol{I} + \left(\nabla_{\boldsymbol{x}} \boldsymbol{v} + \nabla_{\boldsymbol{x}} \boldsymbol{v}^{\mathsf{T}}\right)$, and natural parameter: Reynolds number Re.
"Popular" weak form: find $(\boldsymbol{v}, p) \in \mathbf{V} \times \mathrm{L}^2_0(\Omega)$ such that

$$
\begin{aligned}
Re\ \mathrm{c}(\boldsymbol{v}\,,\, \boldsymbol{v}\,,\, \boldsymbol{u}) + \mathrm{a}(\boldsymbol{v}\,,\, \boldsymbol{u}) + \mathrm{b}(p\,,\, \boldsymbol{u}) &= 0 & \forall \quad \boldsymbol{u} \in \mathbf{H}^1_0(\Omega)\ , \\
\mathrm{b}(q\,,\, \boldsymbol{v}) &= 0 & \forall \quad q \in \mathrm{L}^2_0(\Omega)\ ,
\end{aligned}
$$

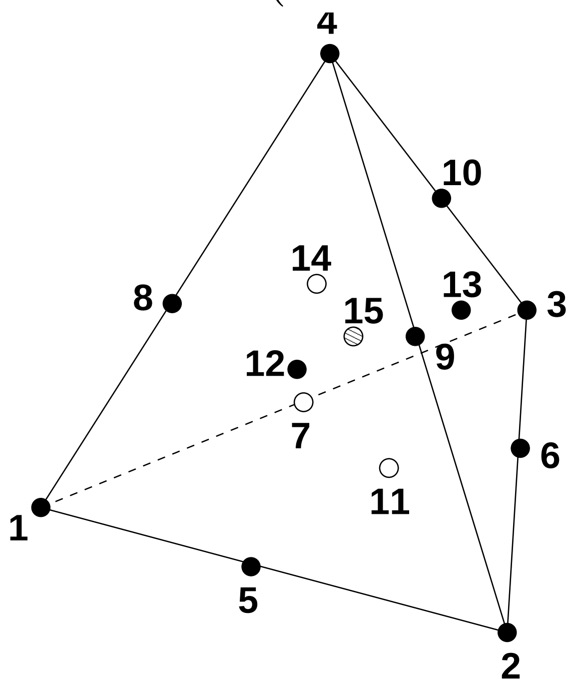
where

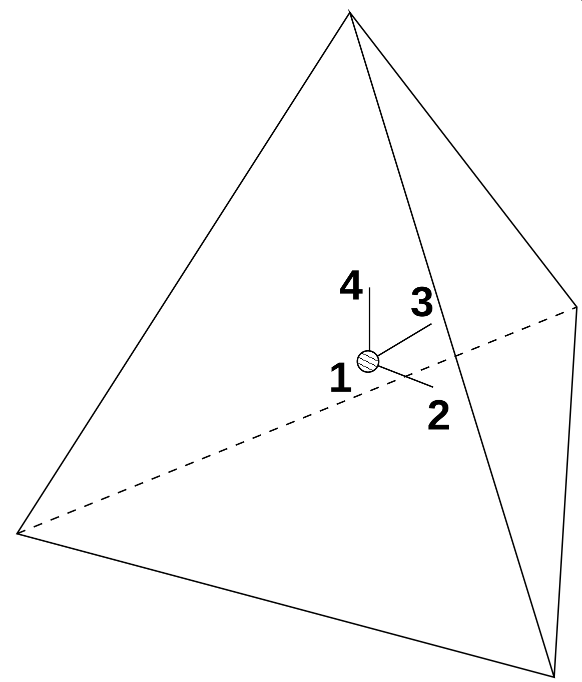
$$
\mathrm{c}(\boldsymbol{w}\,,\, \boldsymbol{v}\,,\, \boldsymbol{u}) := \int_\Omega \nabla_{\boldsymbol{x}} \boldsymbol{w}\, \boldsymbol{v}(\boldsymbol{x}) \cdot \boldsymbol{u}(\boldsymbol{x})\, d\boldsymbol{x}\,,\ \ \mathrm{a}(\boldsymbol{v}\,,\, \boldsymbol{u}) := \int_\Omega \left(\nabla_{\boldsymbol{x}} \boldsymbol{v} + \nabla_{\boldsymbol{x}} \boldsymbol{v}^{\mathsf{T}}\right) \bullet \nabla_{\boldsymbol{x}} \boldsymbol{u}\, d\boldsymbol{x}\,,
$$

$$
\mathrm{b}(p\,,\, \boldsymbol{u}) := \int_\Omega -p(\boldsymbol{x})\, \mathrm{div}_{\boldsymbol{x}} \boldsymbol{u}\, d\boldsymbol{x}\,, \qquad \mathbf{V} := \left\{ \boldsymbol{v} \in \mathbf{H}^1(\Omega) \mid \boldsymbol{v} \equiv \boldsymbol{v}_b \text{ on } \partial\Omega \right\}\ .
$$

TETRAHEDRON P_2^{++}–P_1

VELOCITY (3×15 d.o.f.) DISCONTINUOUS PRESSURE (4 d.o.f.)

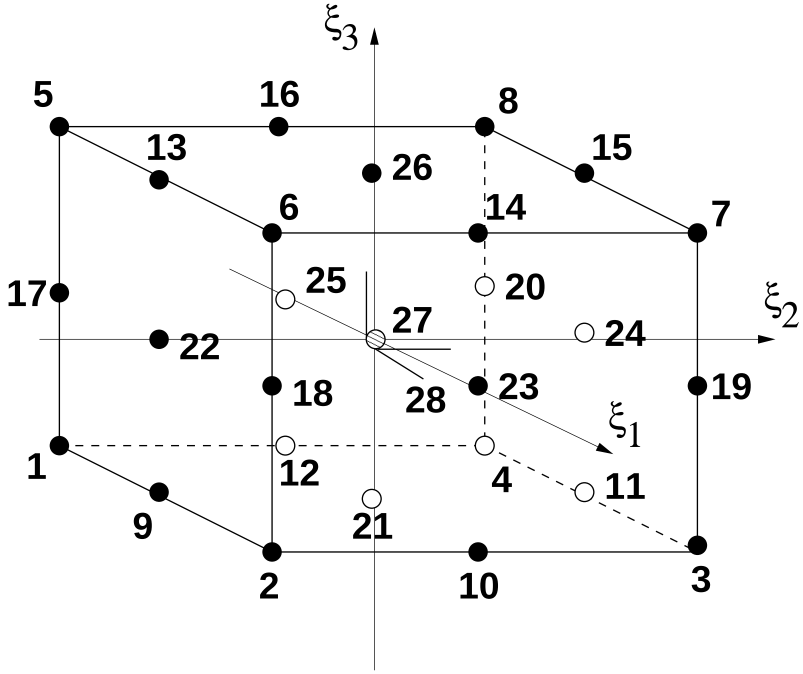




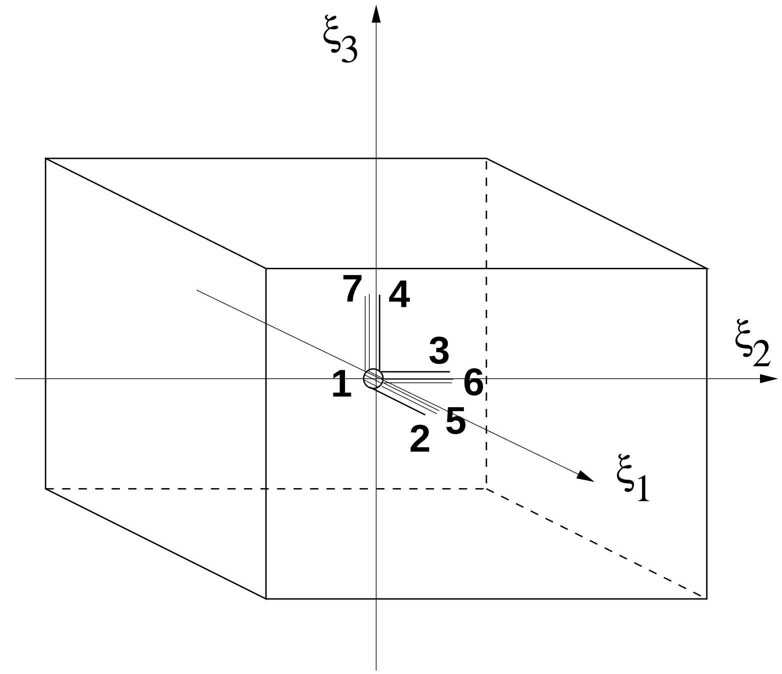
- Based on P_2^{+}–P_1 (Girault and Raviart,1986)
- Second-order accurate. Stable. Elementwise mass conservation
- Data locality allows static condensation of 7 internal degrees of freedom

HEXAHEDRON Q_2^+–P_1^+

VELOCITY $(3 \times 28$ d.o.f.$)$

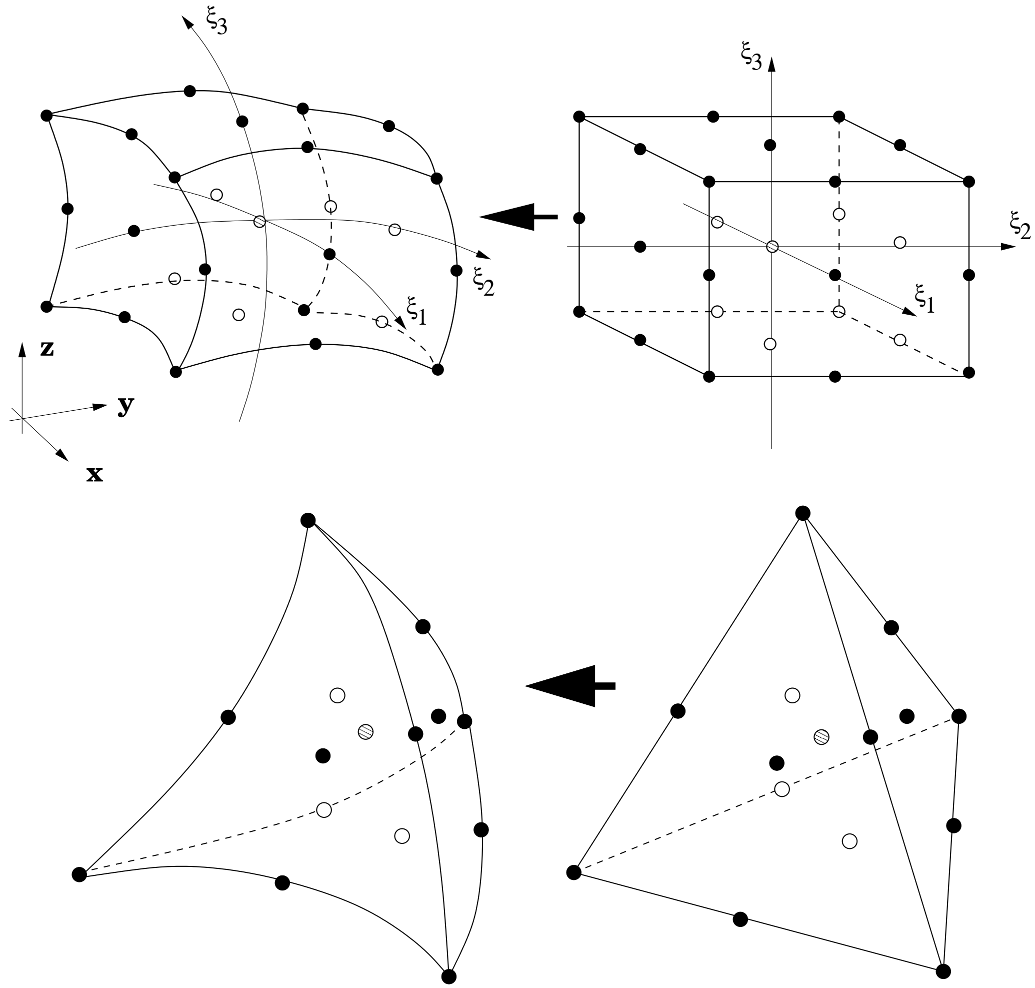


DISCONTINUOUS PRESSURE $(7$ d.o.f.$)$



- Based on Q_2–P_1 (Unknown, 1979)
- Second-order accurate. Stable. Elementwise mass conservation
- Data locality allows static condensation of 13 internal degrees of freedom

ISOPARAMETRIC ELEMENTS

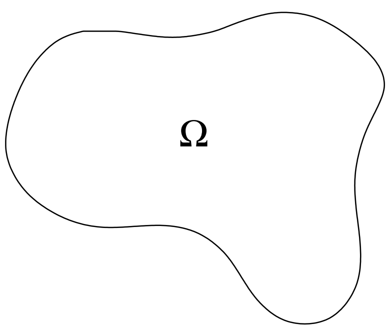


- Can capture geometry curvature with small number of elements

MODIFIED NEWTON-KRYLOV NONLINEAR SOLVER

- Navier-Stokes equations

$$\boxed{\begin{aligned} Re\ \nabla \boldsymbol{v}\, \boldsymbol{v} &= \operatorname{div} \boldsymbol{T} && \text{in } \Omega\ , \\ \operatorname{div} \boldsymbol{v} &= 0 && \text{in } \Omega\ , \\ \boldsymbol{v} &= \boldsymbol{v}_b && \text{on } \partial\Omega\ . \end{aligned}}$$



Reynolds number Re.
Stress tensor
$\boldsymbol{T} := -p\boldsymbol{I} + \left(\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^{\mathsf{T}}\right)$;

- Traditional Newton-like method
  - Given $\boldsymbol{v}^{(0)}$
  - Do $n = 1, 2, 3 \ldots$ (small)
    - Update $\begin{cases} \boldsymbol{v}^{(n)} \equiv \boldsymbol{v}^{(n-1)} + \boldsymbol{v}_c^{(n)}\ , \\ p^{(n)} \equiv p^{(n-1)} + p_c^{(n)}\ . \end{cases}$
    - Solve the linear system

$$\boxed{\begin{pmatrix} \mathsf{A}^{(n-1)} & \mathsf{B}^{\mathsf{T}} \\ \mathsf{B} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{v}_c^{(n)} \\ p_c^{(n)} \end{pmatrix} = \begin{pmatrix} \mathsf{b}_{\boldsymbol{v}}^{(n-1)} \\ \mathsf{b}_p^{(n-1)} \end{pmatrix}}$$

by factorization.

  - EndDo

- Shamanskii's modification (inner iterations)
  - For a given outer iteration n
  - Do $k = 1, 2, 3 \ldots$
    - Update $\begin{cases} \boldsymbol{v}^{(k)} \equiv \boldsymbol{v}^{(k-1)} + \boldsymbol{v}_c^{(k)} \,, \\ p^{(k)} \equiv p^{(k-1)} + p_c^{(k)} \,. \end{cases}$
    - Solve "approximately" the linear system
      $$\boxed{\begin{pmatrix} \mathsf{A}^{(n-1)} & \mathsf{B}^{\mathsf{T}} \\ \mathsf{B} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{v}_c^{(k)} \\ p_c^{(k)} \end{pmatrix} = \begin{pmatrix} \mathsf{b}_{\boldsymbol{v}}^{(k-1)} \\ \mathsf{b}_p^{(k-1)} \end{pmatrix}}$$
      with a preconditioned iterative solver
  - EndDo

- ILUTF(u,tol,$lfil$) GMRES
  - frontal-based incomplete factorization
  - u threshold pivoting
  - tol numerical dropping
  - $lfil$ fill-in cut-off point

OUTLOOK

Suggested improvements towards more realistic modeling

- Parallel computing (possibly terascale)
  - Improved geometry
  - Finer discretization
  - Wider range of parameter study

- Incorporate
  1. Multicomponents
  2. Chemical reactions
  3. Two-phase model