Using CFD to Predict Inspired CO_2 and O_2 after Ventilation Shutoff During a Gateway Emergency Response or Maintenance

ICES 300-A, Paper 402

Marshall McCray

Amentum JETS, Houston, Texas

Rachel Sturtz

Amentum JETS, Houston, Texas

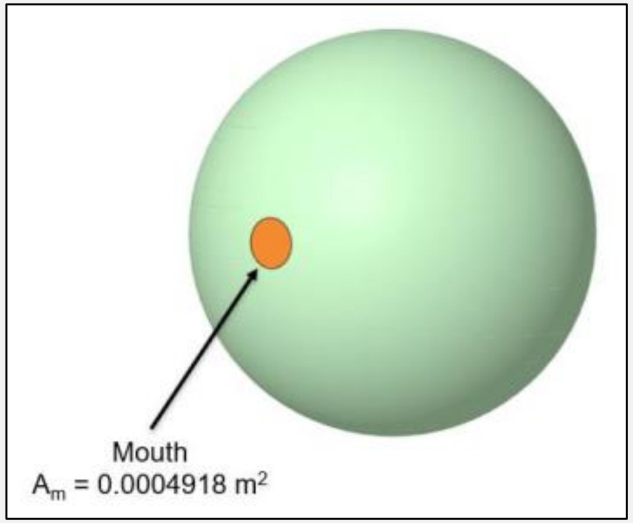
54th International Conference on Environmental Systems, Prague, 13-17 July 2025

Background

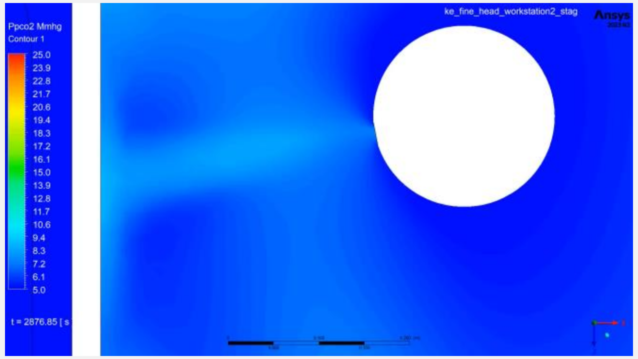
- **Ventilation is important in a crewed space environment because it circulates fresh O_2 to the crew and washes away CO_2**
  - Without ventilation, pockets of low O_2 and high CO_2 can form, posing a hazard to the crew
- **Gateway's Habitation and Logistics Outpost (HALO) provides two forms of ventilation**
  - Intermodule ventilation (IMV): IMV fans exchange air between HALO and adjacent modules
  - Intramodule ventilation: Cabin fans circulate air within HALO to ensure a well-mixed environment
    - Cabin fans also supply air to Air Revitalization System (ARS), which controls temperature, humidity, and removes airborne contaminants
- **However, some off-nominal scenarios require partial or full ventilation shutdown**
  - Fire or chemical spill: fans shut off to prevent flame-feed and limit spread of toxins
  - Leak in pressurized shell: fans shut off so they do not interfere with leak detection
  - Some hardware maintenance tasks may require fans to be off
- **Purpose of CFD analysis: Determine how long crew can remain in a module without ventilation before it harms the crew's health**
  - Assess localized gas concentrations of O_2 and CO_2 near crewmembers
  - Determine time-to-effect for O_2 and CO_2 limits during complete ventilation shutoff

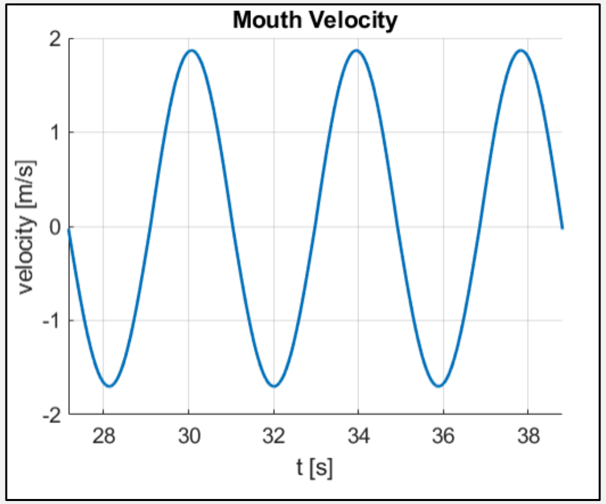
Human Breathing Model

- **Human breathing model**
  - Spherical head, circular mouth
  - Use human test data to convert steady-state metabolic rate (O_2 consumption and CO_2 production) to sinusoidal breathing pattern of constant respiratory rate
  - Inhale: $v(t)$ based on tidal volume, gas concentrations from CFD domain
  - Before exhale, lung species masses are updated: O_2 consumed, CO_2 and H_2O produced, N_2 conserved
  - Exhale: $v(t)$ and species based on updated lung contents



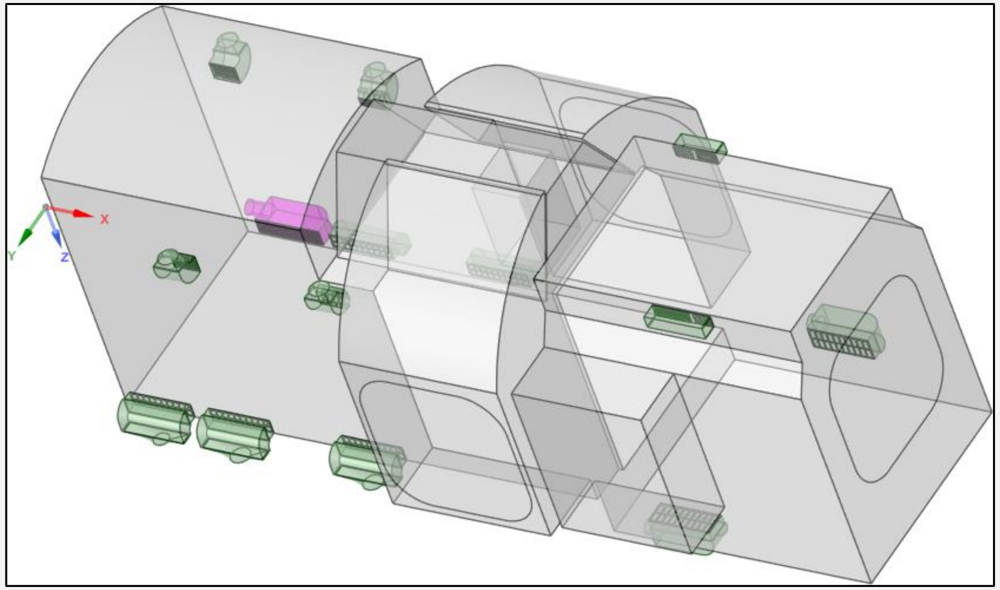
Gender	Male
Aerobic fitness statistic	95%
Metabolic rate	549.5 BTU/hr (161.0 W)
Tidal volume	1.027 L/breath
Respiratory rate	15.49 breaths/min

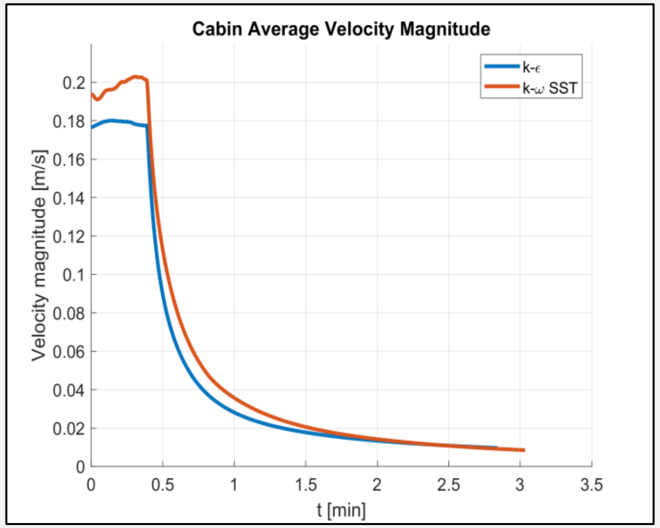


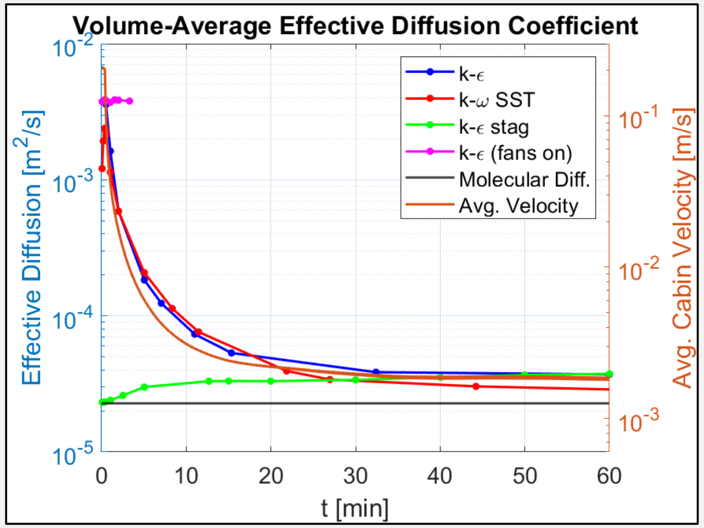


CFD Domain and Boundary Conditions

- **Simplified HALO cabin**
  - Removed ventilation ducting and volumes behind closeout panels to reduce computational effort
  - When fans are on, air enters domain via supply registers (top) and exits via return registers (bottom). Delete vents when fans off.
  - Three ports connect to adjacent modules modeled as flow boundaries based on IMV (120 CFM each)



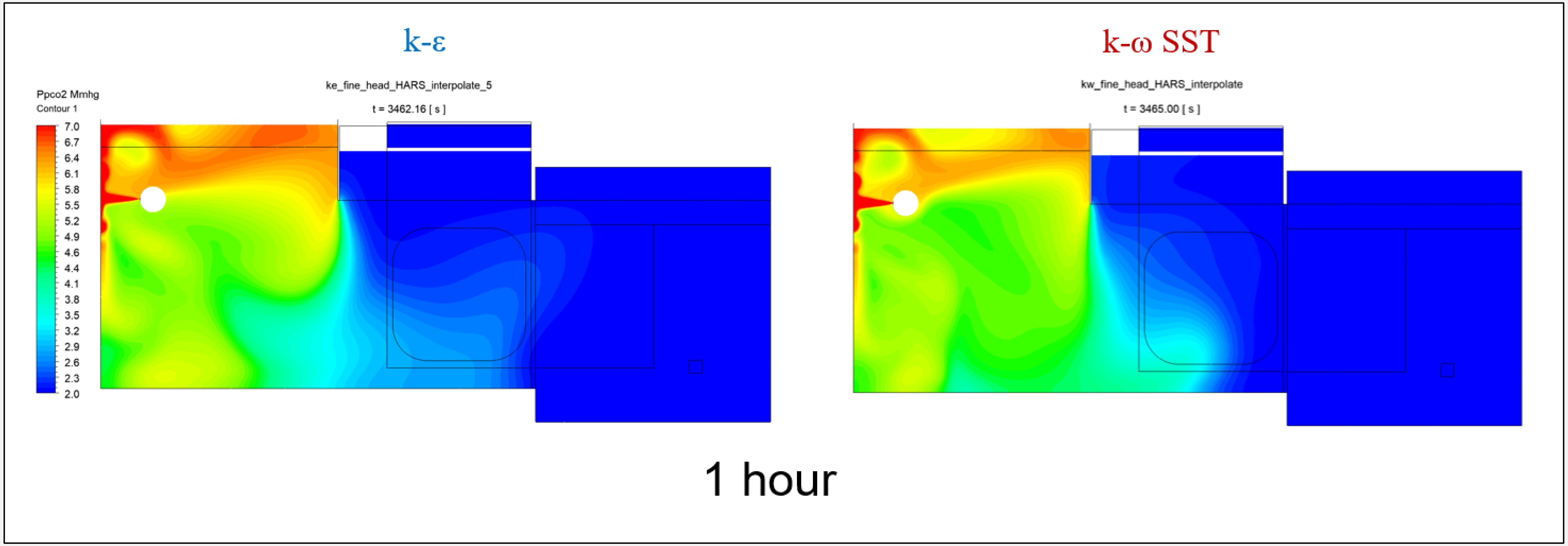




- **Allowed cabin to reach steady-state flow field before ventilation shut off**
  - Ventilation turned off after 23 s
  - Fan-effects fully minimize after ~30 min (diffusion dies down)

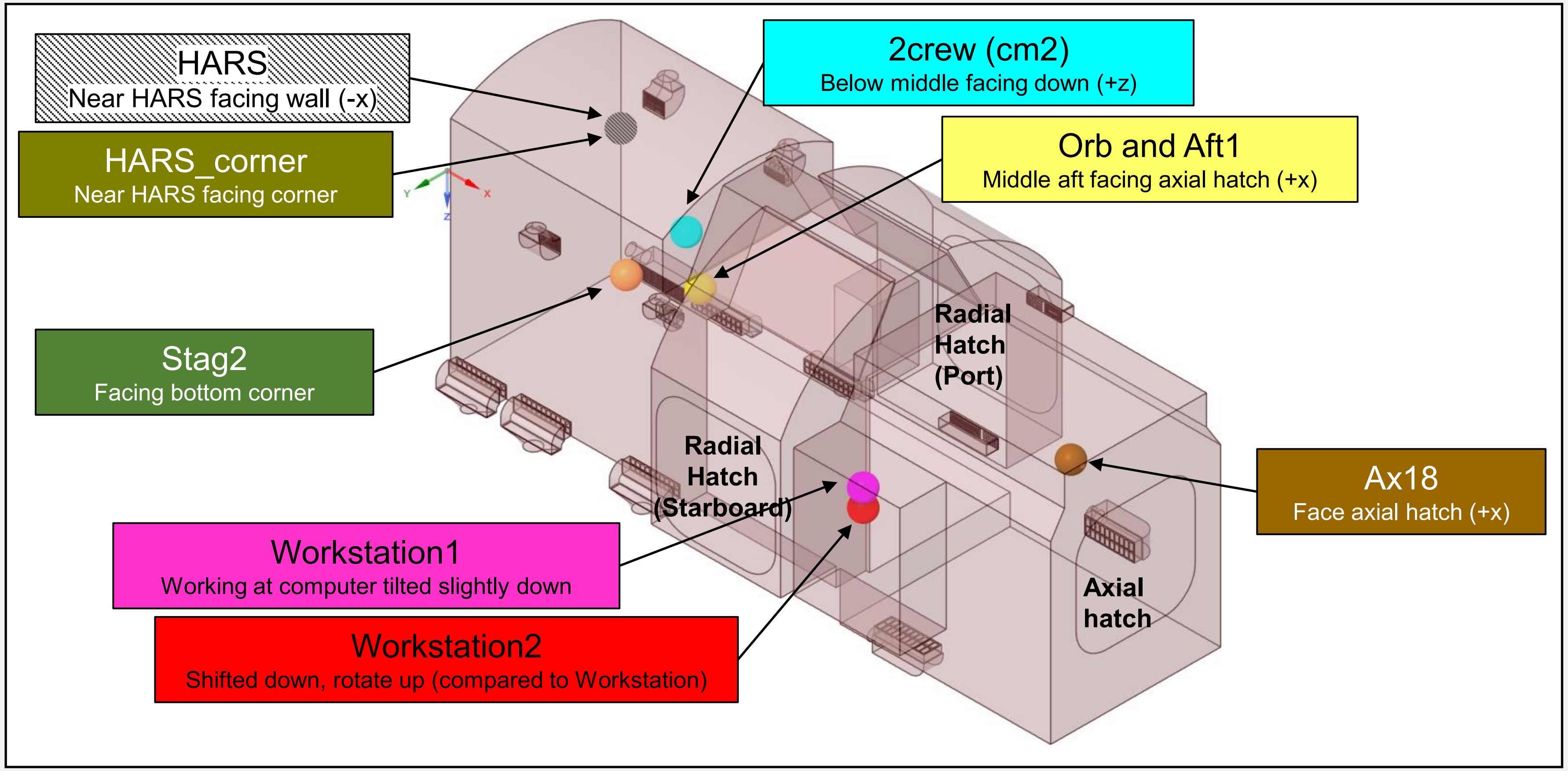
Turbulence model and effect on molecular diffusion

$k-\epsilon$	$k-\omega$ SST
Higer turbulent kinetic energy	Lower turbulent kinetic energy
More diffusion	Less diffusion
Lower concentration CO_2 pockets	Lower concentration CO_2 pockets
Longer time-to-effect	Shorter time-to-effect



Crewmember Location

- **Simulated a range of crewmember breathing locations to evaluate if it impacted time-to-effect**
  - Simulated one or two crewmembers in the module at one time
  - Used awake metabolic rate for all crewmembers

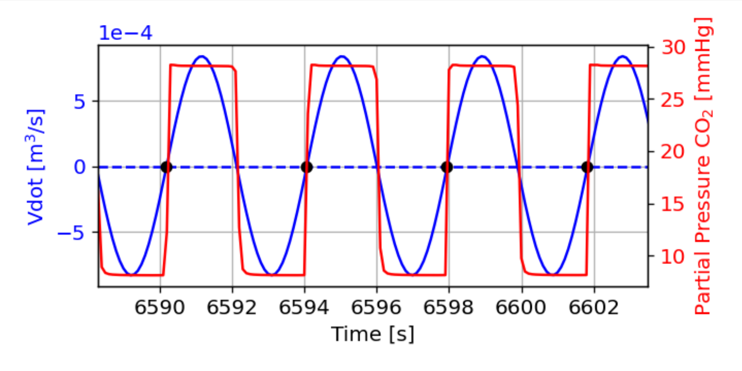


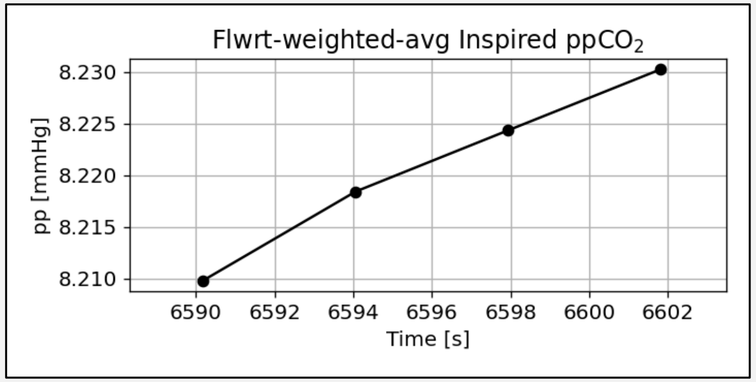
Concentration Limits and Time-to-effect

- **Crew requires minimum partial pressure of 127 mmHg inspired O_2**
- **For CO_2, maximum exposure times are defined based on concentration:**

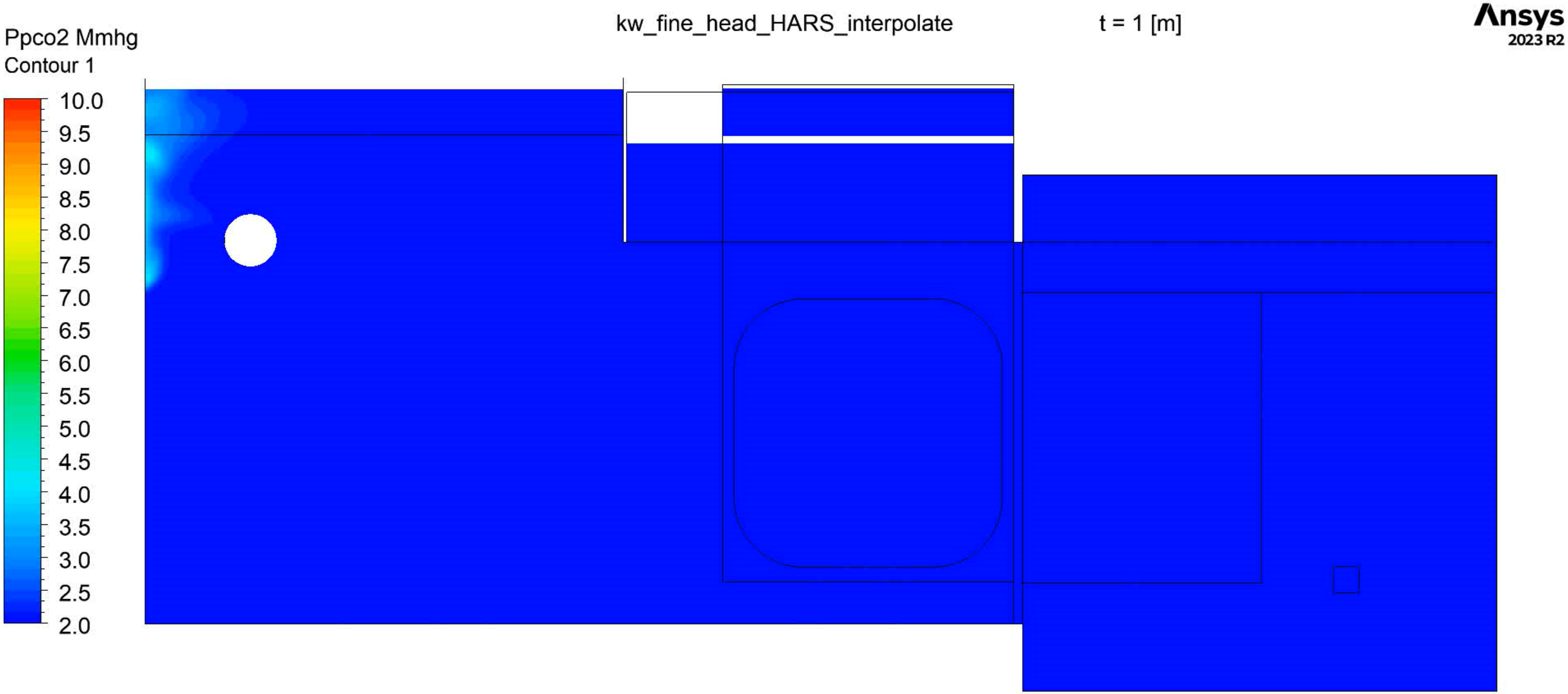
$ppCO_2$ (kPa)	$ppCO_2$ (mmHg)	Exposure Time
0 - Nominal	0 - Nominal	Indefinite
Nominal - 0.9	Nominal - 6.8	8 hours
0.9 - 1.3	6.8 - 10	4 hours
1.3 - 2.0	10 - 15	1 hour

- **Time-to-effect: the time before either one of these limits is exceeded**
- **To evaluate the crewmember's exposure, calculate flow-rate-weighted-average inspired partial pressures at mouth surface for each inhale:**





Preview (2 hr timelapse)

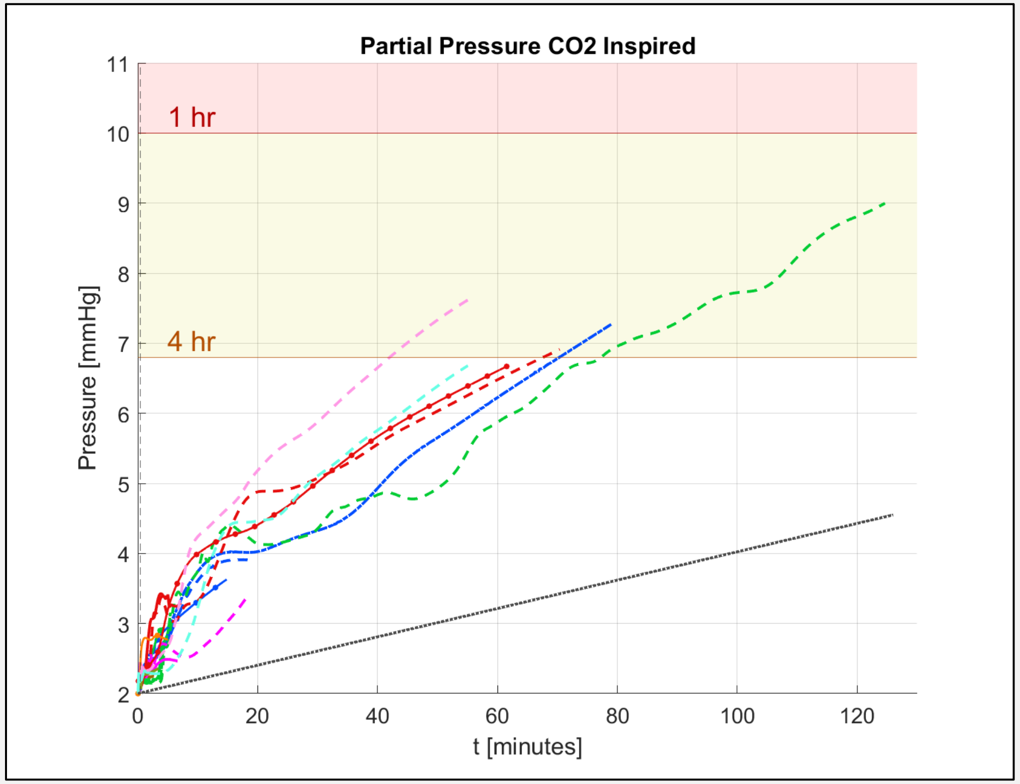


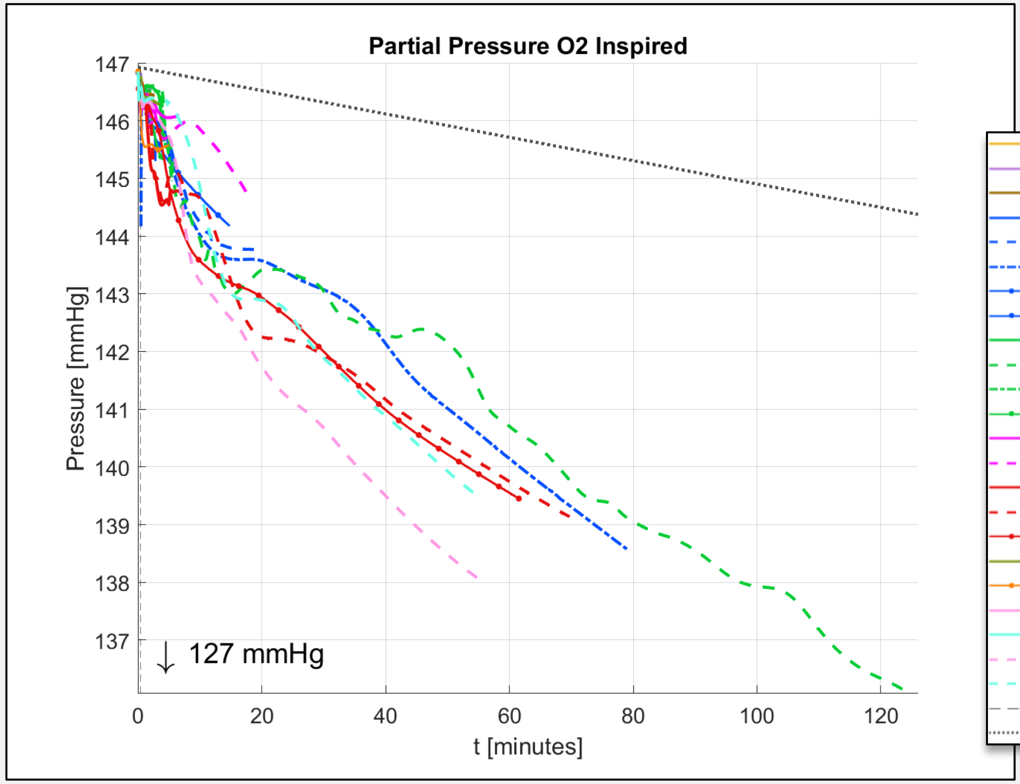
Results

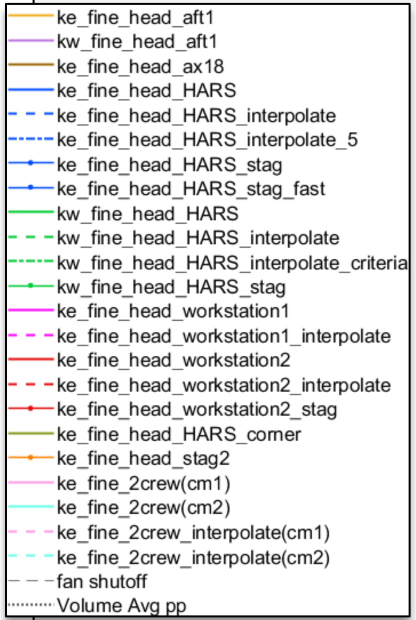
- **All results**
  - Over time, the CO_2 accumulates as the O_2 depletes, with inhaled $ppCO_2$ exposure limit exceeded first

$ppCO_2$ (mmHg)	Exposure Time
0 - Nominal	Indefinite
Nominal - 6.8	8 hours
6.8 - 10	4 hours
10 - 15	1 hour

ppO_2: 127 mmHg

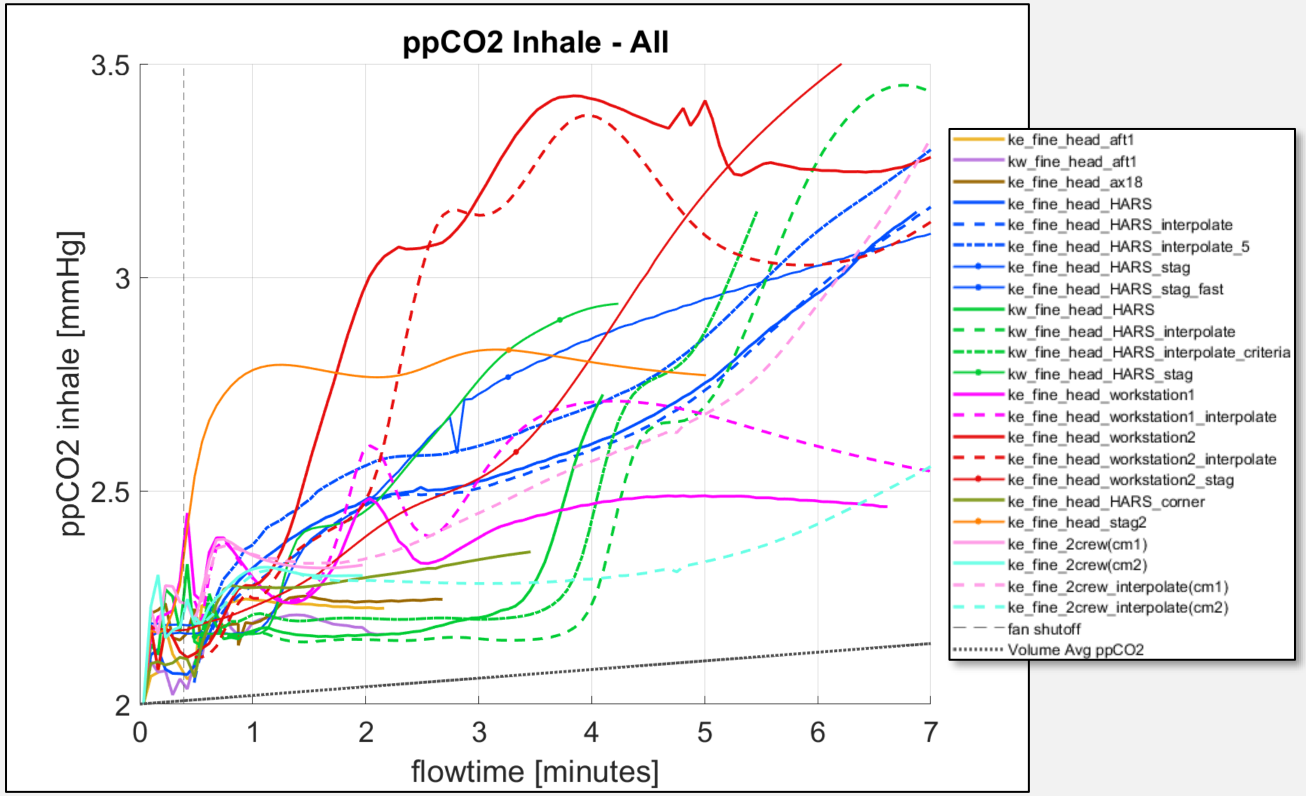


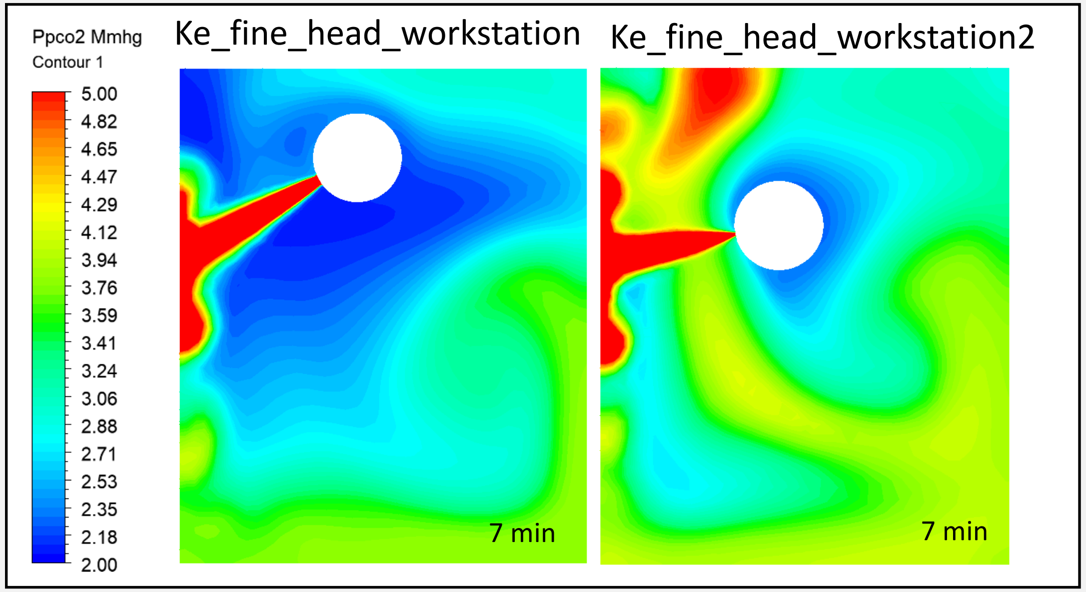




Results – Short Term

- **Short-term CO_2 inspired results (< 7 minutes)**
- **Highly dependent on breathing location and turbulence model**
- **All results comfortably within nominal CO_2 range**





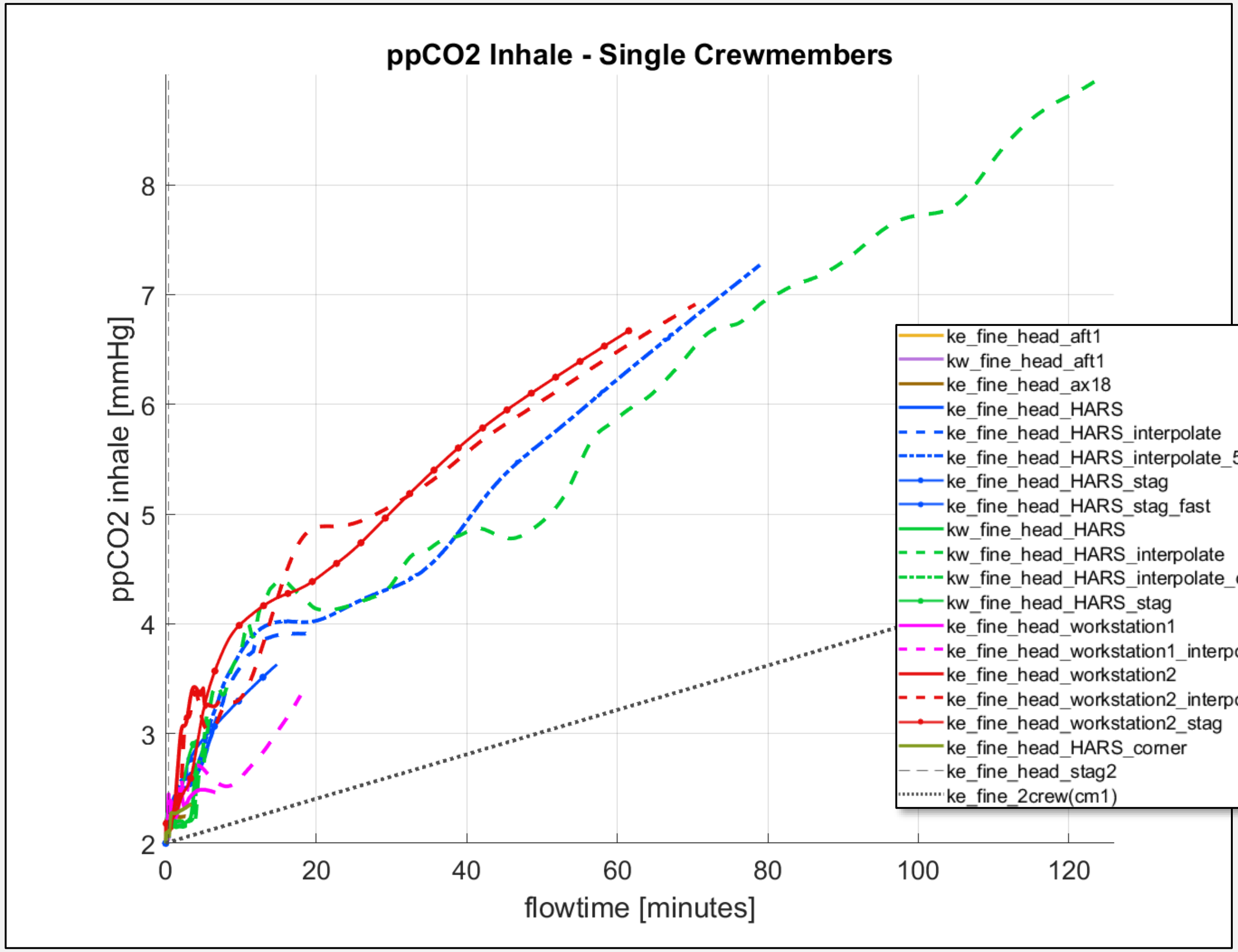
$ppCO_2$ (kPa)	$ppCO_2$ (mmHg)	Exposure Time
0 - Nominal	0 - Nominal	Indefinite
Nominal - 0.9	Nominal - 6.8	8 hours
0.9 - 1.3	6.8 - 10	4 hours
1.3 - 2.0	10 - 15	1 hour

Results – Long-Term

- **< 30 minutes**
  - High variance for breathing location and turbulence model
- **> 30 minutes**
  - Rate CO_2 inhaled similar regardless of location and turbulence model
  - Similar slopes of CO_2 inspired at 1 hour

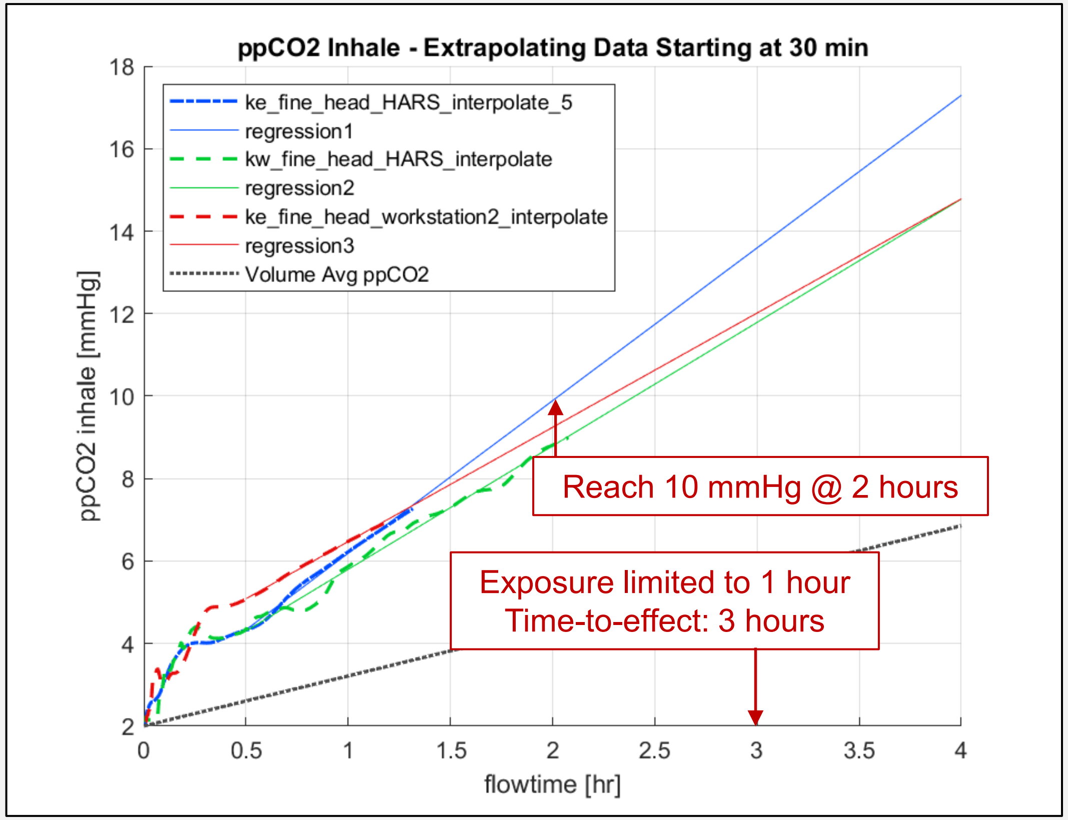
$ppCO_2$ results [mmHg]	
t	Single Crew
5 min	2 - 3.5
15 min	3.0 - 4.6
30 min	4.3 - 5.1
1 hr	5.8 - 6.6

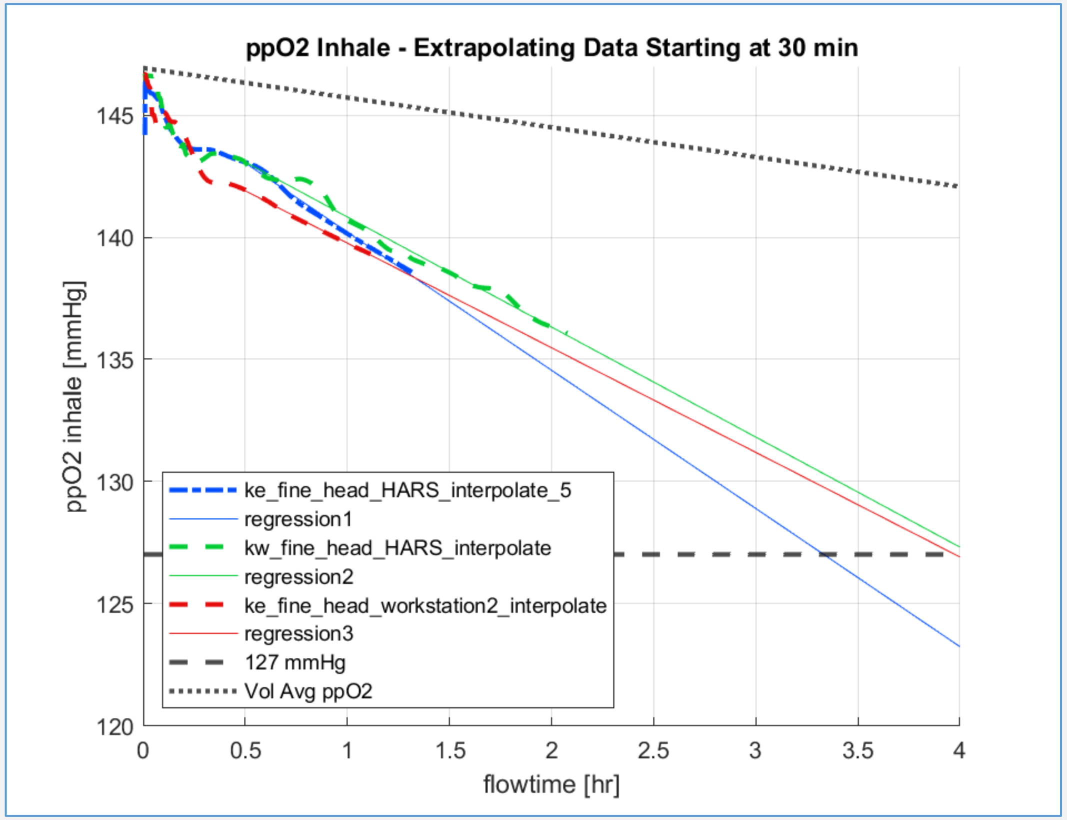
$ppCO_2$ (kPa)	$ppCO_2$ (mmHg)	Exposure Time
0 - Nominal	0 - Nominal	Indefinite
Nominal - 0.9	Nominal - 6.8	8 hours
0.9 - 1.3	6.8 - 10	4 hours
1.3 - 2.0	10 - 15	1 hour



Estimate Time-to-Effect by Extrapolating Regression

- **Extrapolate linear regression (data > 30 min) to estimate time-to-effect**





Estimated Time-to-Effect $ppCO_2$

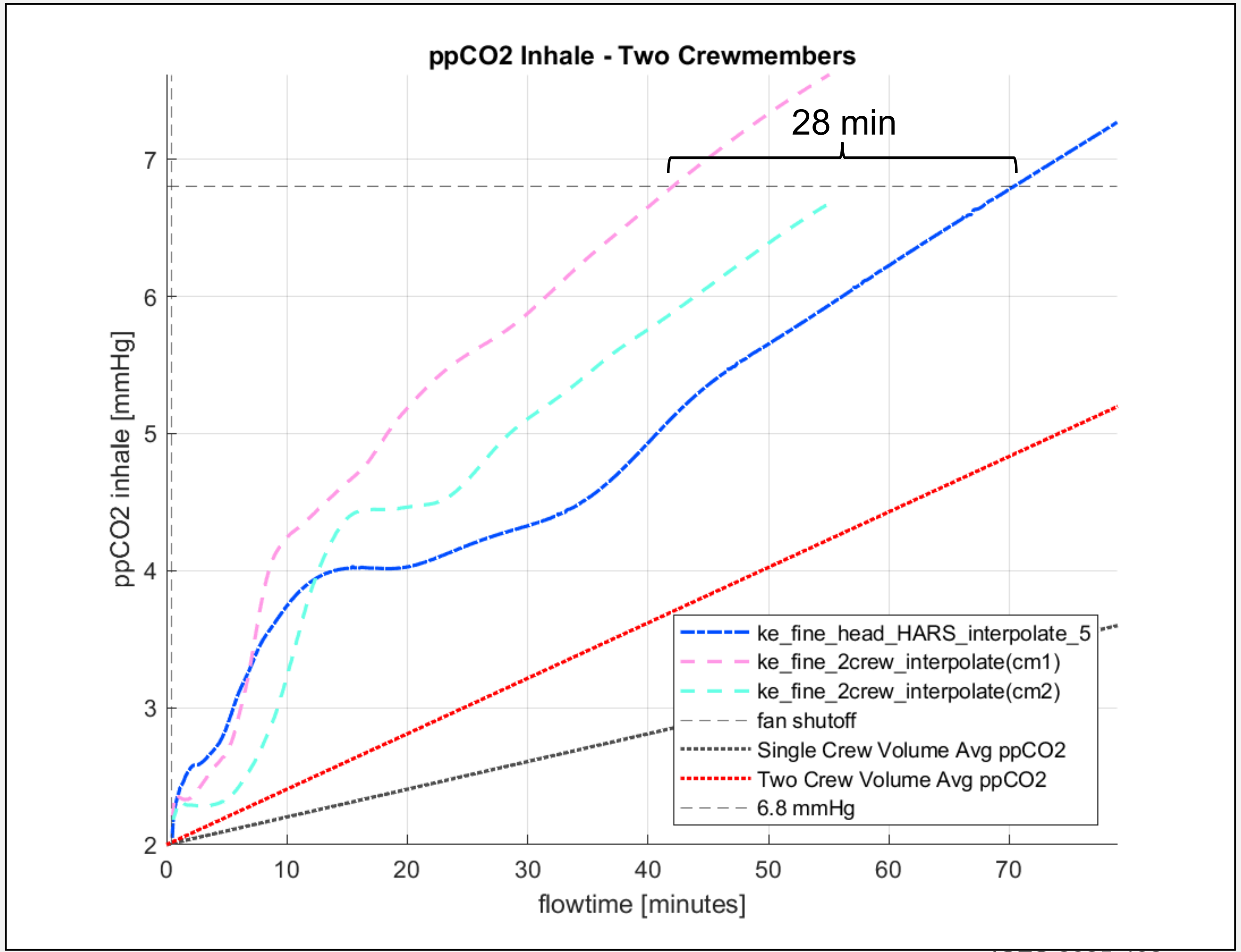
$ppCO_2$	Time to Reach Specified $ppCO_2$	Exposure Time Allowed	**Time to Max Exposure limit**
6.8 mmHg	1.0 hr	8 hours	**9 hr**
10 mmHg	2.0 - 2.4 hr	1 hour	**3.0 - 3.4 hr**
15 mmHg	3.4 - 4.1 hr	none	**3.4 – 4.1 hr**

Estimated Time-to-Effect ppO_2

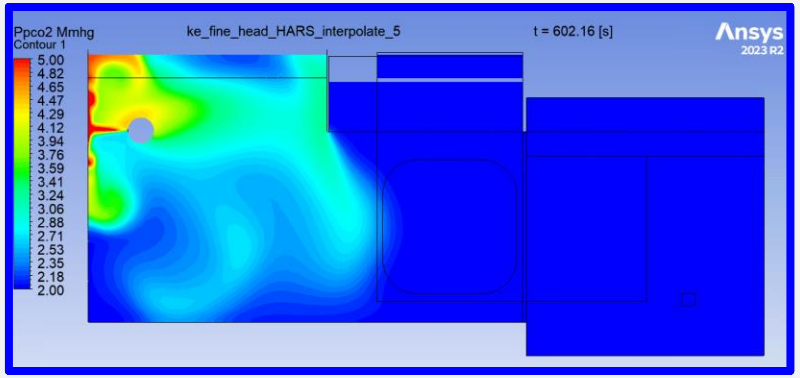
ppO_2	Time to Reach Specified ppO_2
127 mmHg	3.25 - 4 hr

Results – Two vs One Crewmember(s)

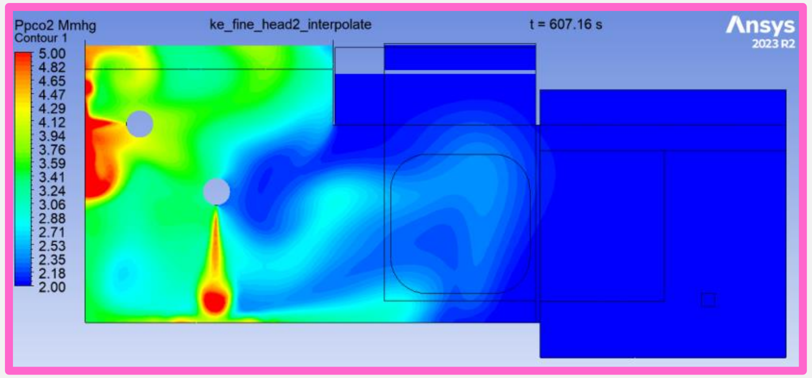
- **Added second crewmember nearby to evaluate impact**
  - Note: only one dual-crew breathing case tested



- **Royal blue: single crew case**

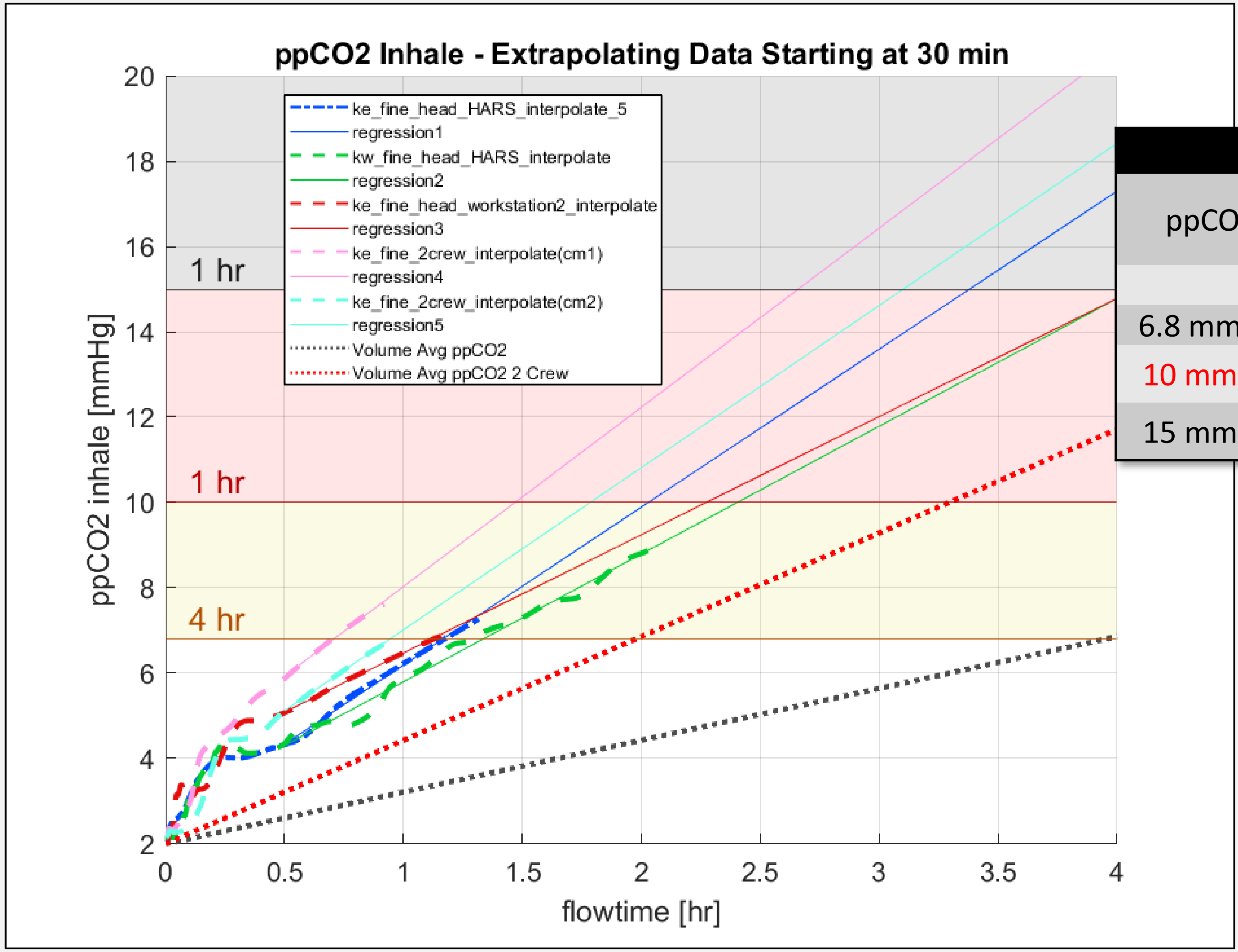


- **Pink: Crewmember #1 at same location**
- **Cyan: Crewmember #2 nearby**



Results – Extrapolated Time-to-Effect Estimates

- **Adding second crewmember reduced time-to-effect from 3 hr to 2.4 hr**



Estimated Time-to-Effect $ppCO_2$

$ppCO_2$	Time to Reach Specified $ppCO_2$		Exposure Time Limit	**Time to Max Exposure limit**	
	Single Crew	Two Crew		Single Crew	Two Crew
6.8 mmHg	1.0 hr	40 mins	8 hours	**9 hr**	**8.7 hr**
10 mmHg	2.0 - 2.4 hr	1.4 - 1.8 hr	1 hour	**3.0 - 3.4 hr**	**2.4 – 2.8 hr**
15 mmHg	3.4 - 4.1 hr	2.6 - 3.1 hr	none	**3.4 – 4.1 hr**	**2.6 – 3.1 hr**

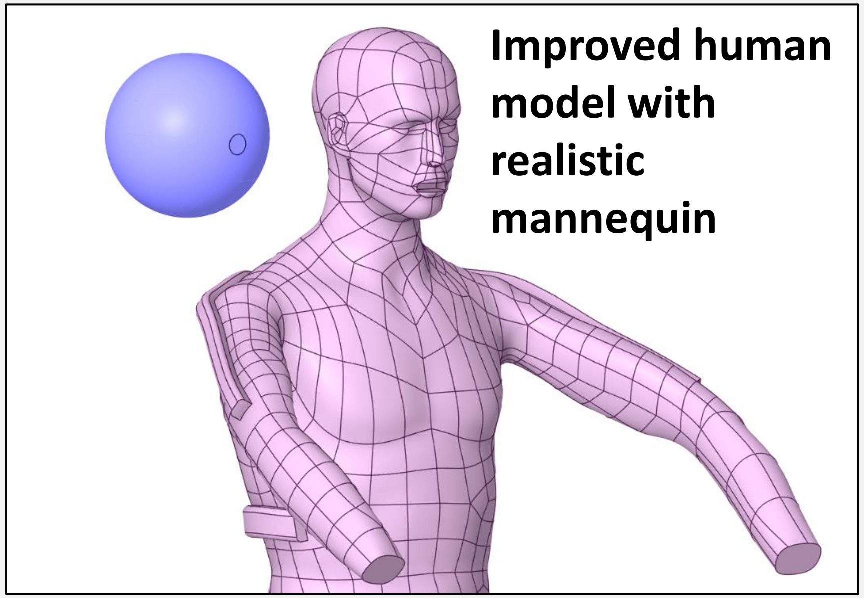
Estimated Time-to-Effect ppO_2

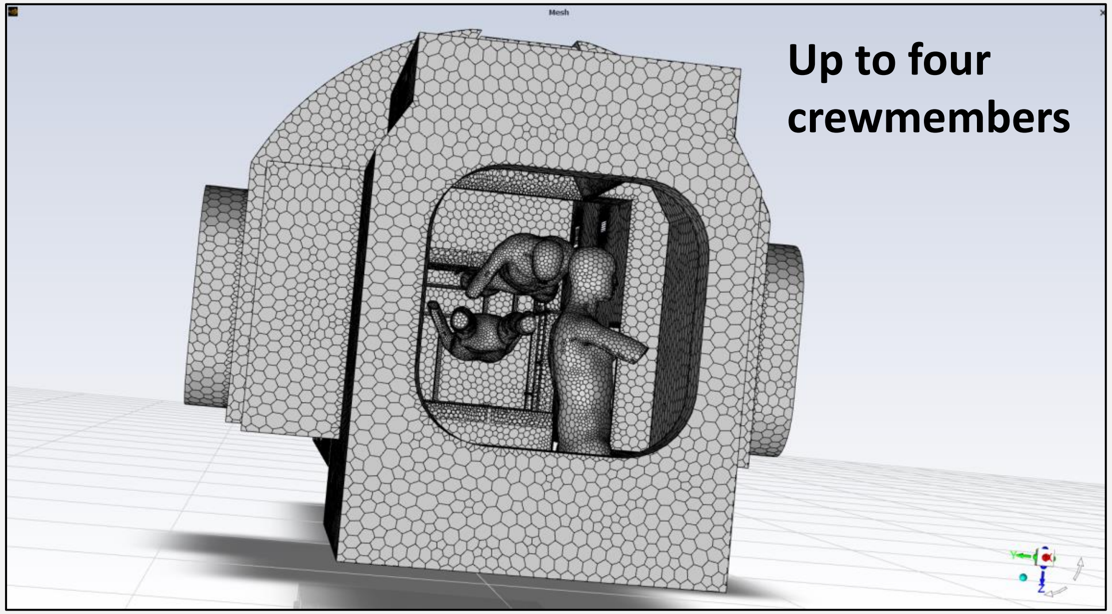
ppO_2	Single Crew	Two Crew
127 mmHg	3.3 - 4.1 hr	2.6 - 3.0 hr

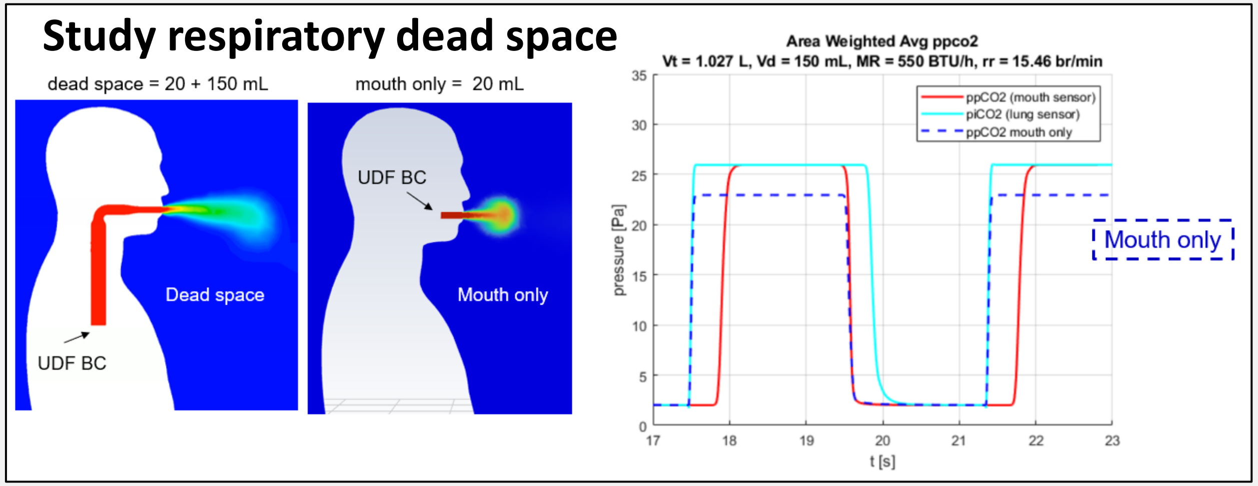
Conclusions

- **The results of this CFD analysis help inform how long a crewmember can safely work in a module without ventilation and provide analytical data for defining flight rules**
- **In all cases analyzed, the exposure limit for CO_2 was exceeded before O_2 concentrations dropped below the minimum limit**
- **Both the breath plume's momentum and species diffusion affect localized CO_2 buildup**
  - When fans are off, most of the air movement is caused by the crewmembers breathing
  - Breathing angle and nearby surfaces impact how local CO_2 concentrations accumulate
- **Important to model human with directional mouth (as apposed to a "point source" type of geometry, which will result in unrealistically high CO_2 inspired)**

Forward Work





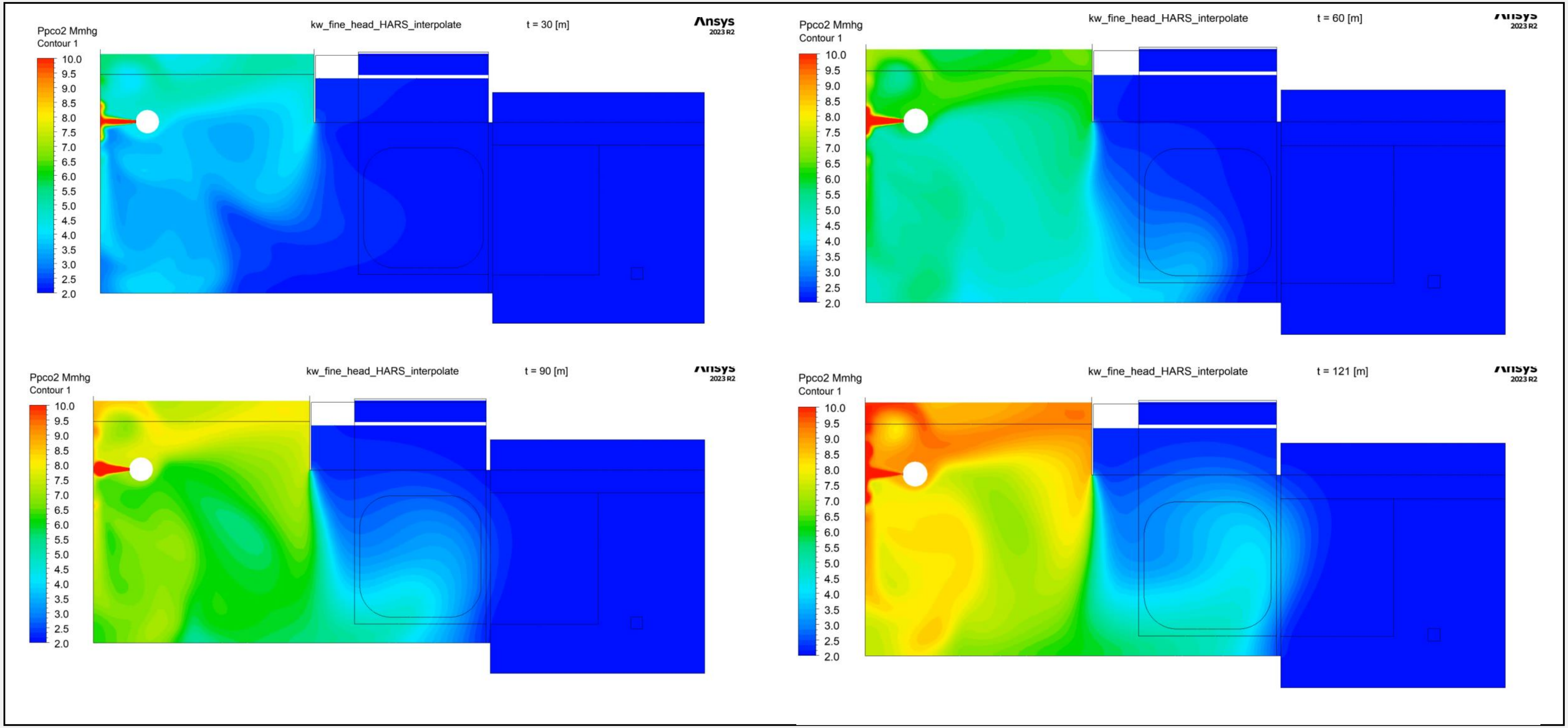


Questions?

Backup

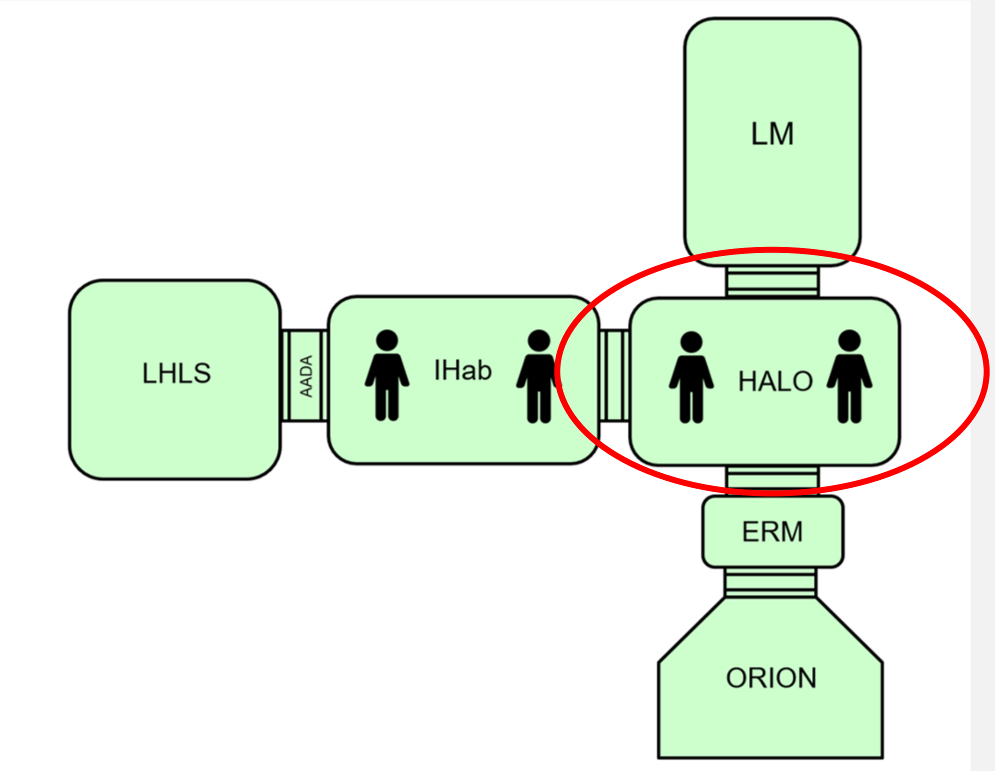
CO_2 Buildup over time

- $ppCO_2$ contours at 30, 60, 90, and 120 minutes



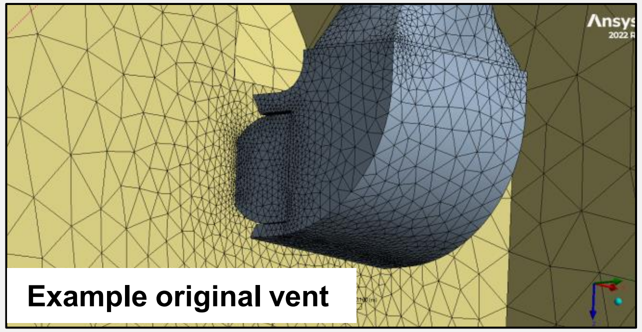
HALO Geometry Overview and Ventilation Assumptions

- **Integrated Gateway Stack**
  - HALO CFD analysis is *not* stack specific
    - Assumes modules are docked on all three of HALO's ports
    - Does *not* factor in which modules are docked to HALO's three ports

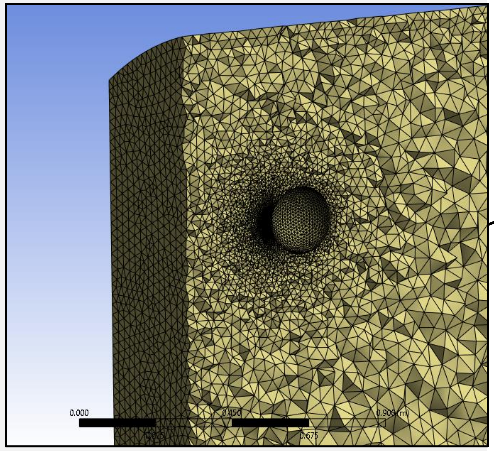


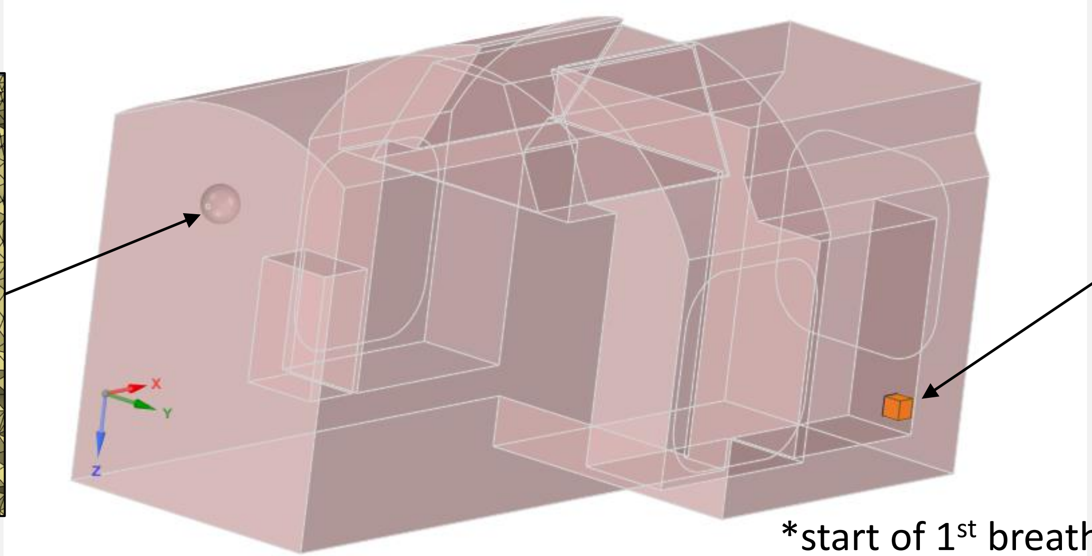
Removing Vents

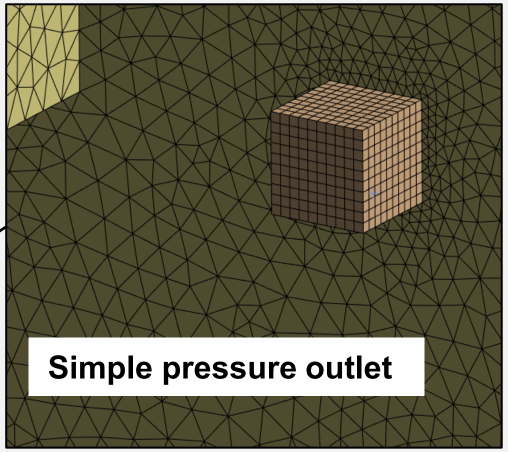
- **Vents account for 75% of mesh cell count and are not relevant after fans shut off**
  - Vents only account for 0.68% of the combined volume
- **Delete vents to reduce cell count (9.1M tet / 2.8M poly → 2.5M tet / 462K poly)**
  - One simple pressure outlet for numerical stability
    - Reversed flow mass fractions from volume average in cube
  - Example case from 27.16s* to 244.44s (3.6 min simulation):
    - With vents (kw_fine_head_HARS) → 4.3 days
    - Deleted vents (kw_fine_head_HARS_interpolate) → 1.1 days
  - Bonus: mesh quality increased slightly (max skewness from 0.85 to 0.75)



Example original vent



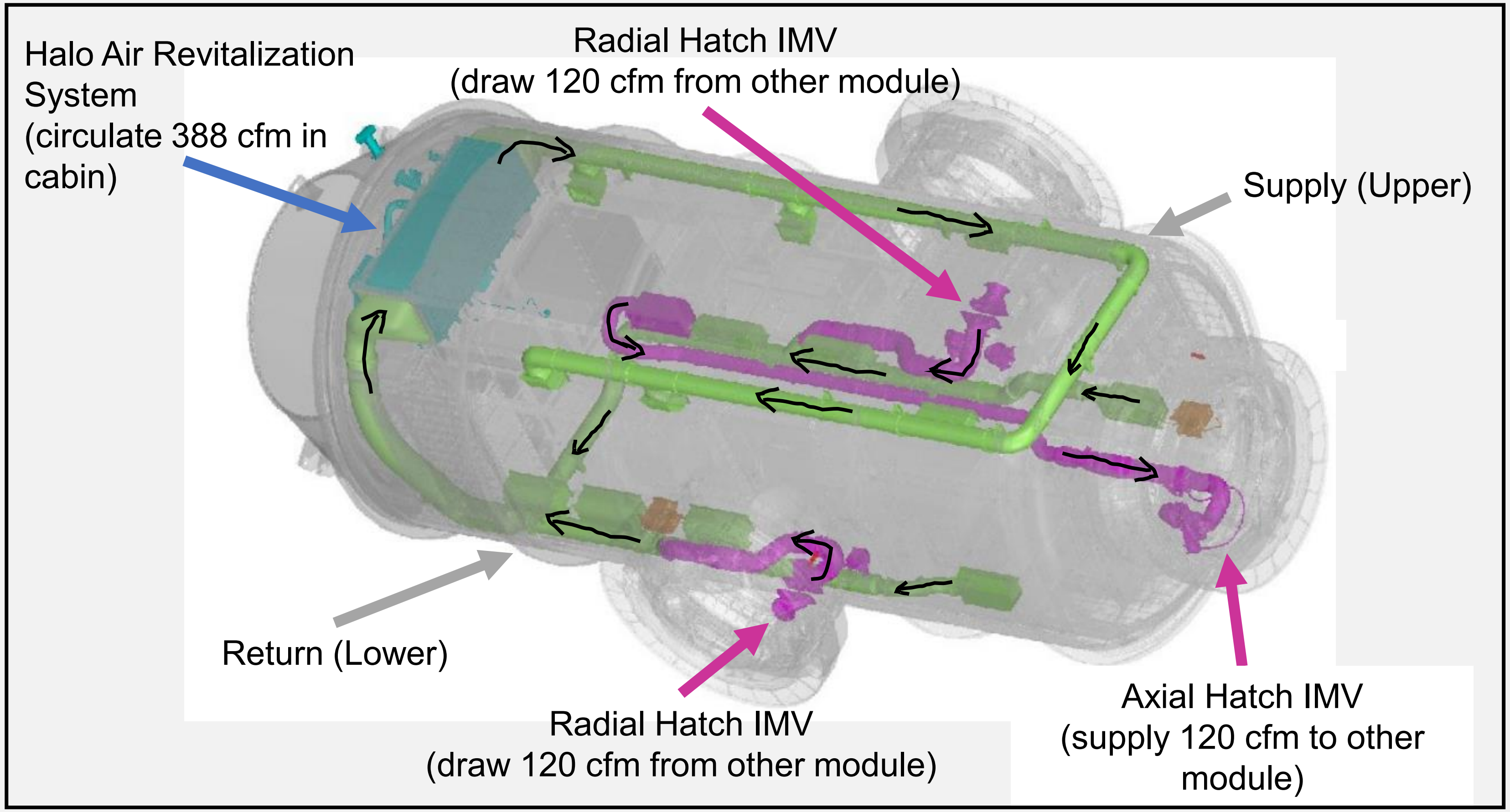



Simple pressure outlet

*start of 1st breath period after fans off

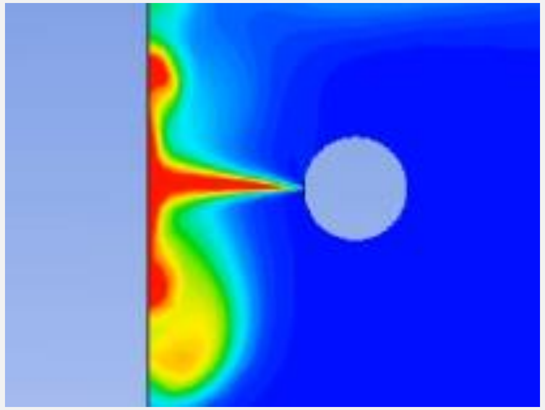
HALO Geometry Overview and Ventilation Assumptions

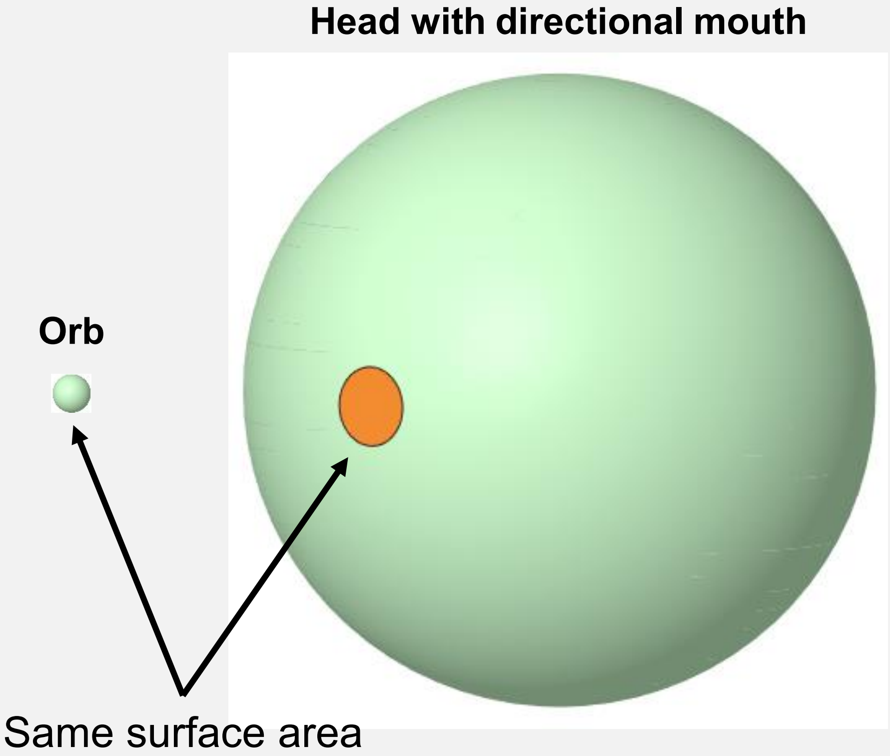
- **Intra-modular ventilation (fans circulate cabin air) [green]**
- **Inter-module ventilation (fans move air to/from other modules) [pink]**
- **Accounted for loop flow-rates, but not included in CFD model**



Crew Modeling Approaches – Orb mouth vs Directional Mouth

- **Crew modeling approaches**
  - Mouth modeled as orb or head with directional mouth
  - Detailed human body not included
  - Mouth area (orb and mouth) from suit model ≈ 0.0004918 m^2
  - Assume circular mouth for directional breathing model → D ≈ 1 inch
  - Breath temperature = 310 K (98.3 F)
  - Max Re = 1700





Crew Modeling Approaches – Metabolic Rate

- **Metabolic rate (95th percentile male, awake) ← GP-10004**
  - Nominal awake metrate = 549.5 [BTU/hr]
  - CO_2 production = 0.8058 [g/min]
  - O_2 consumption = 0.6810 [g/min]
  - H_2O mass exhaled → pV = nRT (vapor pressure H_2O, lung volume, amount H_2O, gas constant, breath temp.)
- **Use test data to determine respiratory rate and tidal volume**
  - Minute volume = 16 [L/min] (total volume inhaled per minute)
  - Respiratory rate* = 15.46 [breaths/min] (results in 3.88s breath period)
- **Fluent User Defined Function (UDF) ← how model interprets that**
  - Fluent breathing UDF developed by M. Navarro and B. Conger for suit analysis
  - Takes minute volume, respiratory rate and mouth area and converts to sinusoidal velocity profile with constant amplitude and period

Updated data from Jason Norcross 2022 (50% male).
95% male was determined by increasing tidal volume by 16%
Ref. [JETS-JE33-22-TLSS-DOC-0032]

Metrate BTU/hr	Minute volume [L/min]	Tidal Volume (50% male) [L/breath]	Respiratory Rate (50% male) [Breath/min]	Tidal Volume (95% male) [L/breath]	Respiratory Rate (95% male) [Breath/min]
500	15.05	0.85	18.84	0.99	15.26
1000	24.64	1.21	20.52	1.40	17.55
1500	33.31	1.68	20.91	1.95	17.09
2000	45.89	2.09	22.7	2.42	18.93
2500	62.37	2.45	25.88	2.84	21.95
3000	82.77	2.75	30.44	3.19	25.95

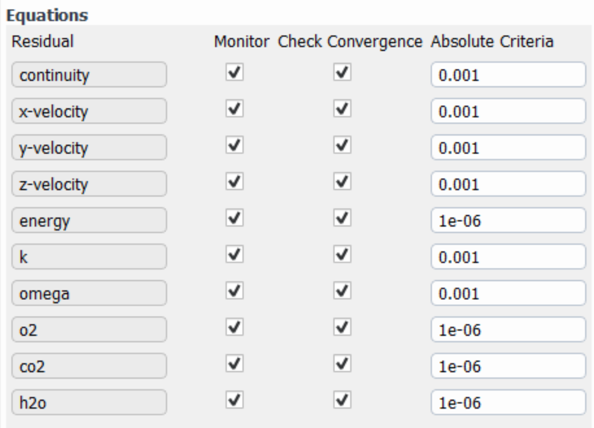
Links metrate to breath volume and rhythm using human test data

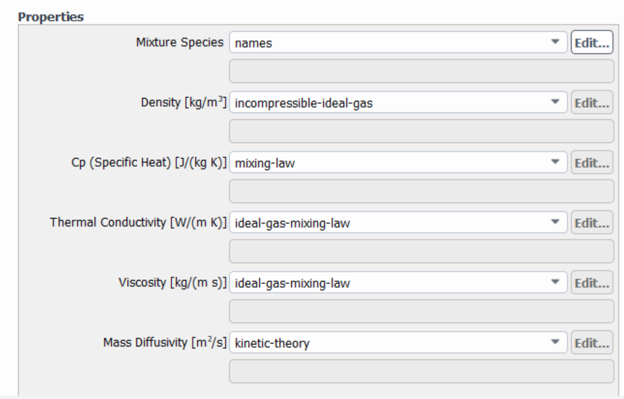
metrate 95	550	BTU/hr
tidal volume 95	1.031	L/breath
rr 95	15.489	br/min
mv 95	15.96916	L/min

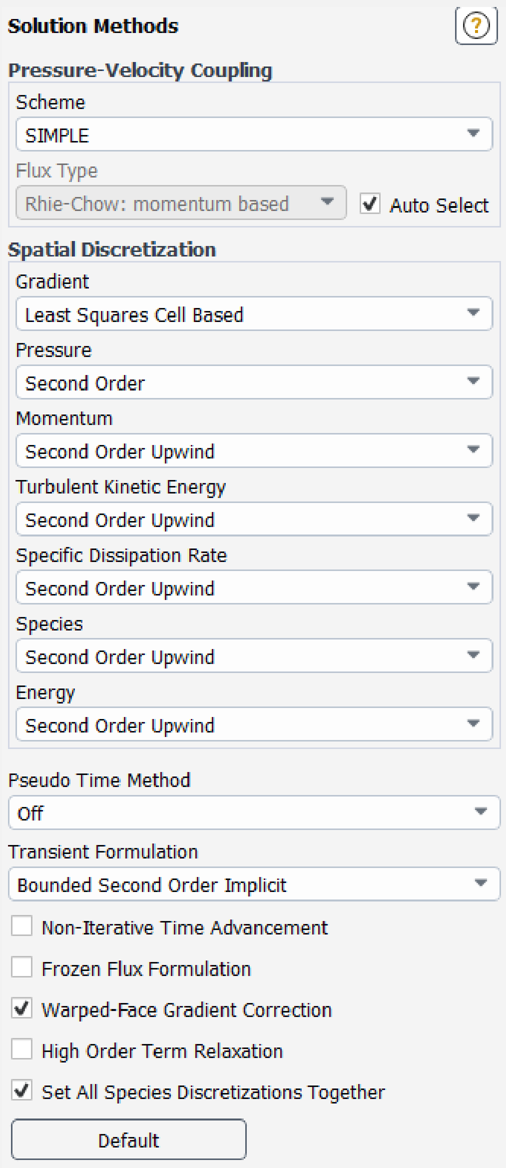
* Use a breath period that is perfectly divisible by the timestep so that autosaves can happen exactly at the beginning of each breath period. Restarts should occur at the beginning of the breath period since re-compiling the UDF causes the initialization of mass fractions exhale = 0. In the future, the mass fraction exhale for each species should be written to a file so that restarts could happen at any timestep.

CFD Model – Main

- **Reynolds-averaged Navier Stokes (RANS)**
  - Time-averaged effects of turbulence are modeled
- **Pressure-based solver**
  - SIMPLE pressure-velocity coupling
- **2nd Order discretization**
- **Incompressible ideal gas**
  - Pressure gradients negligible, fluid density function of temperature only
- **Species transport model**
  - Non-reacting
- **Time-stepping**
  - dt = 0.01s (usually), implicit bounded 2nd order
- **Convergence conditions set to default (or stricter)**
- **Standard wall functions for turbulence models**

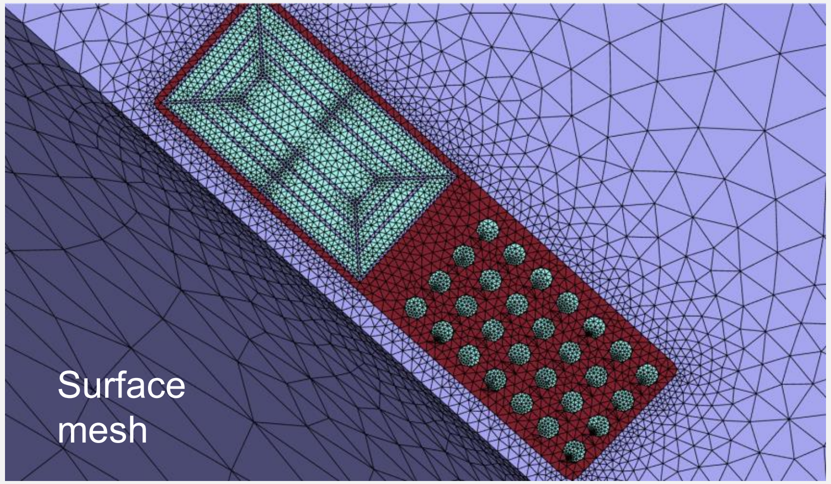


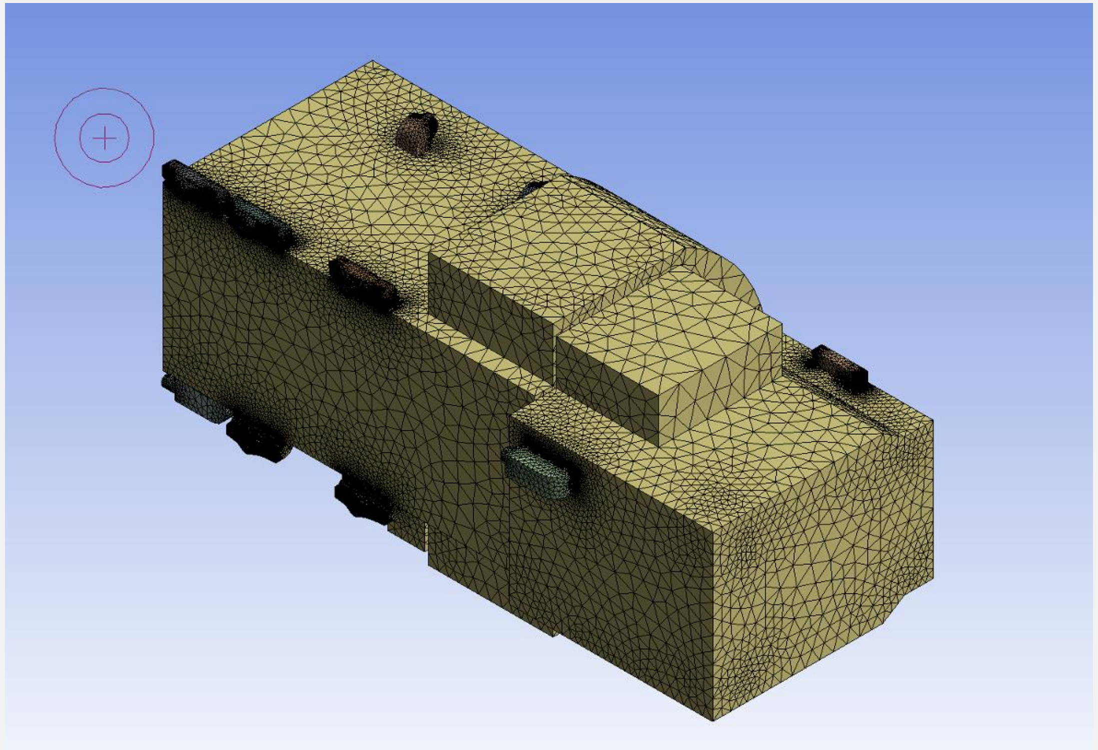




Mesh

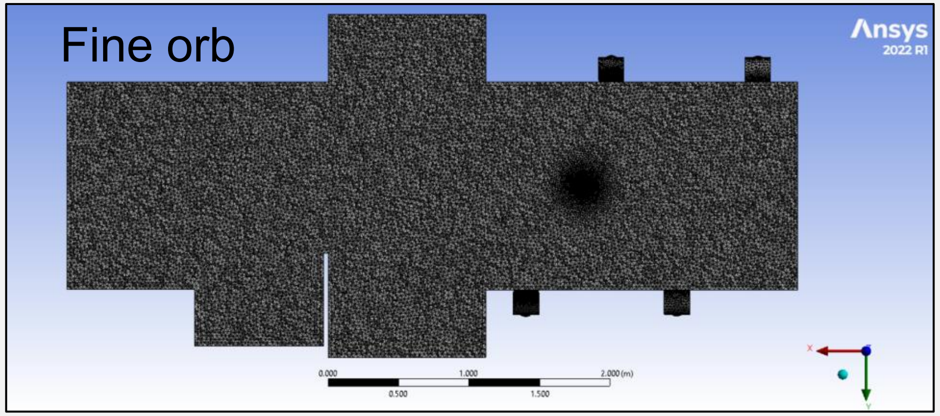
- **Mesh**
  - Discretize flow domain into finite number of cells
  - Solve governing equations (x8) in each cell
    - Density, pressure, 3D velocity, temperature, two turbulence variables
  - Too coarse → poor accuracy
  - Excessively fine → slow simulation
  - Other mesh metrics
    - Skewness, gap factor

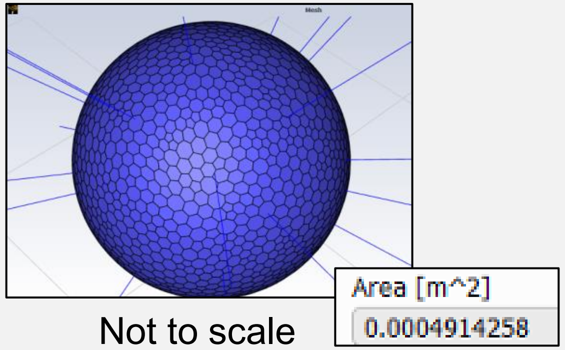




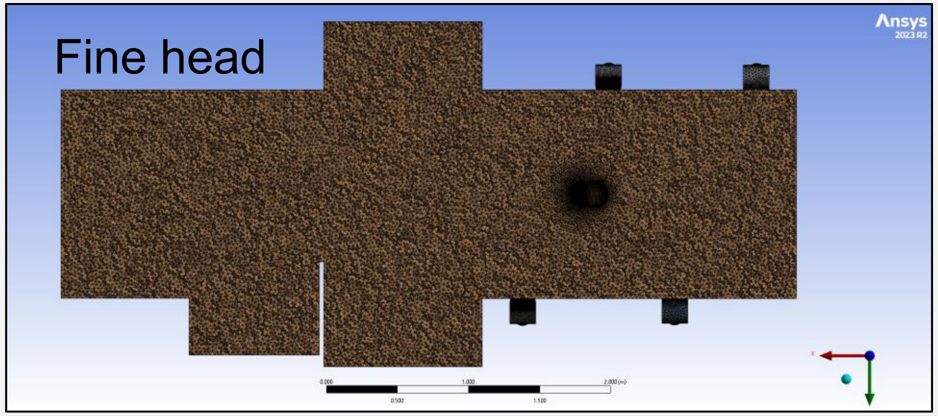
Mesh Settings – Orb vs Directional

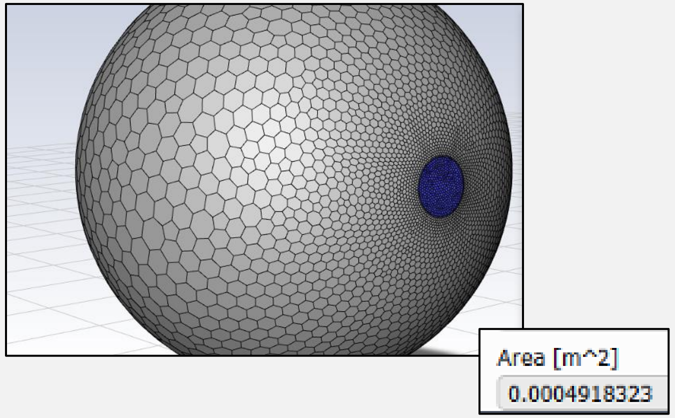
- **Mesh settings applied to both breathing geometries**
  - 9.1M tetrahedral / 2.1M polyhedral (compare to 8.3 / 2.3 fine orb)
  - Max skewness: 0.85





Not to scale





Mesh settings

Mesh Name	copyfine
Defaults	
Element size	6.10E-02
Sizing	
Use Adaptive Sizing	No
Growth Rate	1.2
Max Size	6.10E-02
Defeature Size	3.05E-04
Capture Curvature	Yes
Curvature Min Size	6.10E-04
Curv Normal Angle	89
Capture Proximity	Yes
Proximity Min Size	3.00E-03
Prox Gap Factor	1.8
Prox Size Sources	Fcs & Edgs
Quality	
Target Skewness	0.9
Smoothing	High
Inflation	
Use Auto Inflation	None
Inflation Option	Smth Tran
Transition Ratio	0.272
Maximum Layers	20
Growth Rate	1.2
Inflation Algorithm	Pre
Mouth Face Sizing	
Mouth Face Element Sz	1.00E-03
Mouth Defeature Sz	1.00E-05
Mouth Influence Vol	No
Mouth Behavior	Soft
Mouth Growth Rate	1.08
Mouth Capture Curv.	no
Mouth Curv norm Angl.	-
Mouth Capture Prox.	no
Mouth local min size	-

Head Face Sizing	
Head Face Element Sz.	1.00E-02
Head Defeature Sz.	3.05E-04
Head Influence Vol.	No
Head Behavior	Soft
Head Growth Rate	1.2
Head Capture curvature	No
Head Curv norm angle	-
Head Capture Prox.	No
Head local min size	-
Cabin Volume Sizing	None
Element Size Cabin	3.00E-02
Defeature Size Cabin	3.05E-04
Growth Rate Cabin	1.2
Capture Curv Cabin	no
Cabin Curv. Norm. Angl.	-
Cabin Local Min Size	-
Capture Prox Cabin	no
Prox Min Size Cabin	-
Prox Gap Factor Cabin	-
Results	
Nodes	12.5
Elements tet/poly	9.05
Min Element Quality	
Max Aspect Ratio	
Max Skewness	0.85
Min Orth Quality	
Min edge length	
Generate time (10 proc)	

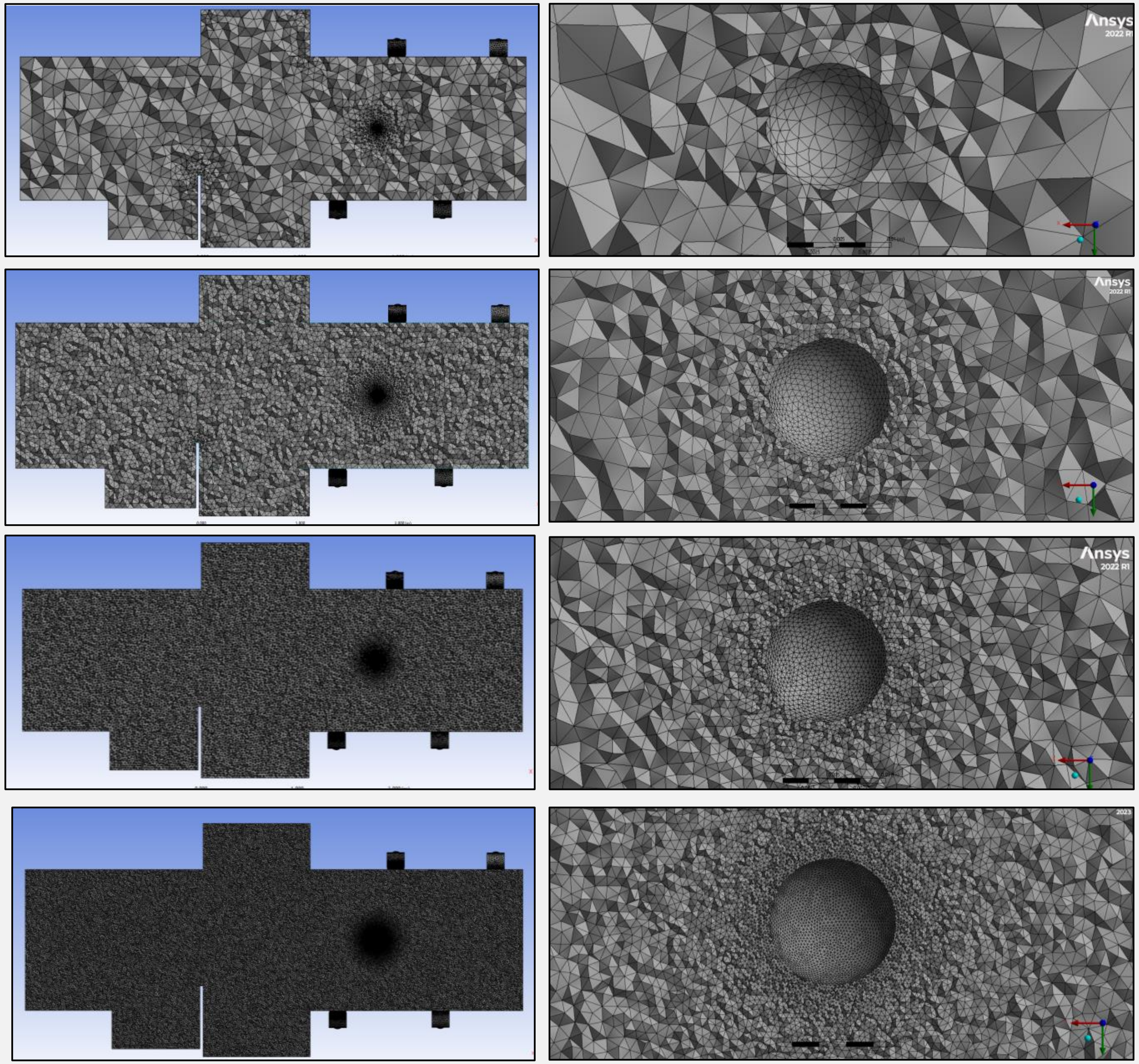
Mesh Refinement Study

Coarse
2.96M Tetrahedral
0.97M Polyhedral

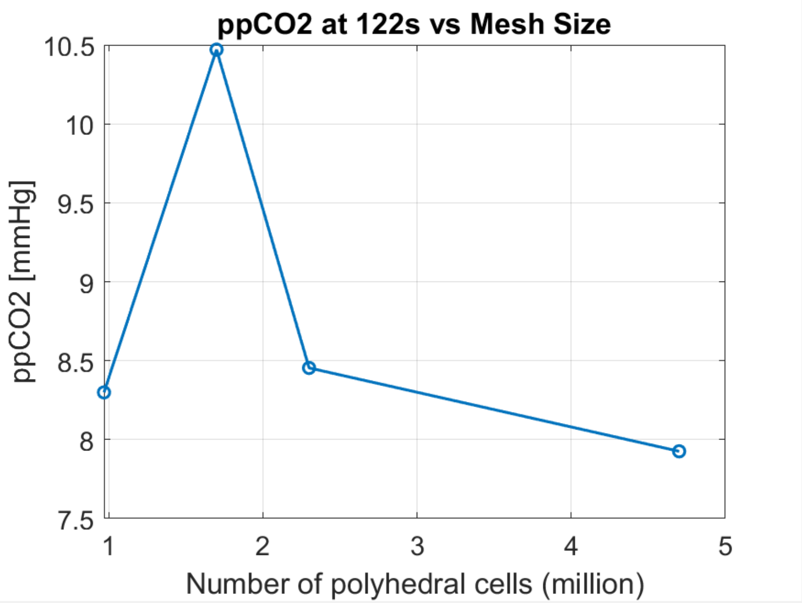
Medium
5.6M Tetrahedral
1.7M Polyhedral

✓ **Fine**
8.26 M Tetrahedral
2.3M Polyhedral

XL
22.3M Tetrahedral
4.7M Polyhedral

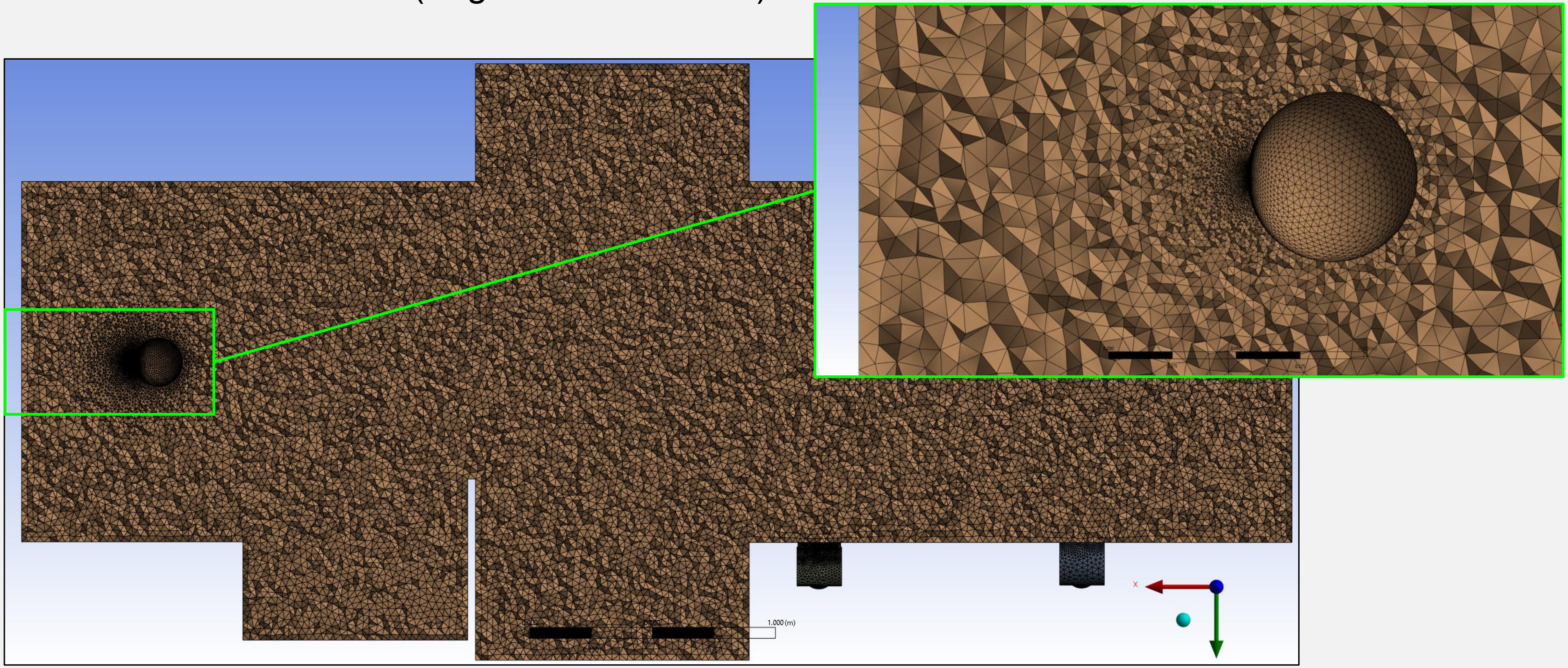


- Goal: find coarsest mesh that does not significantly compromise accuracy
- Mesh selected when further refinement does not significantly change solution
- k-ε turbulence model + orb geometry, middle aft location



Mesh Settings – Location

- **Meshes are generated with same settings, regardless of crew location**
  - Cell count: 9.8M tetrahedral / 2.8 polyhedral (vents included)
  - Max skewness = 0.85 (target 0.9 and below)



CFD Model Workflow – Interpolated Cases (Fast)