by B.C. Lyons¹, C.C. Kim², J. McClenaghan¹, P.B. Parks¹, L.L. Lao¹

¹ General Atomics ² SLS2 Consulting

1

Presented at the SciDAC Center for Tokamak Transient Simulation Group Meeting Princeton, NJ, USA April 14th, 2019



M3D-C1 Impurity-MHD Modeling B.C. Lyons, N.M. Ferraro, S.C. Jardin



M3D-C1 Extended-MHD Solver Coupled to KPRAD

M3D-C1* solves the extended-MHD equations

- 3D toroidal geometry
- Full (not reduced) MHD
- High-order finite-element representation in (R, ϕ , Z)
- Two-fluid effects (optional)
- Finite-thickness resistive wall (optional)

• Recently coupled⁺ to KPRAD[‡] for impurity-plasma interactions

- Coronal (non-equilibrium) model
- Impurity charge states and electron density evolve according to ionization and recombination
- Thermal energy loss (ionization and radiation) coupled to
 - One (total) or two (total & electron) pressure equations
 - One (all-species) or two (all-ion and electron) temperature equations
- Subcycled much faster than typical MHD time steps

* S. C. Jardin, et al., Comput. Sci. Discovery 5, 014002 (2012).
† N.M. Ferraro et al. Nucl. Fusion 59 016001 (2019).
‡ D.G. Whyte, et al., Proc. of the 24th Euro. Conf. on Controlled Fusion and Plasma Physics, Vol. 21A, p. 1137 (1997).

M3D-C1 and NIMROD* Coupling to KPRAD Successfully Benchmarked in Axisymmetric Simulations

- Both codes solved same problem of impurity injection into DIII-D core
 - DIII-D shot 137611 @ 1950 ms
 - 2D, nonlinear, single-fluid
 - Single-temperature equation
 - Fixed boundary
 - Constant injection of neutrals in Gaussian centered on-axis
- Quantitative agreement found in
 - OD time histories
 - 2D contours
 - Temperature
 - Current



- *C. R. Sovinec et al., J. Comput. Phys. 195, 355 (2004).
- C. Sovinec & J. King, J. Comput. Phys. 229, 5803 (2010).

M3D-C1 and NIMROD Coupling to KPRAD Successfully Benchmarked in Axisymmetric Simulations

- Both codes solved same problem of impurity injection into DIII-D core
 - DIII-D shot 137611 @ 1950 ms
 - 2D, nonlinear, single-fluid
 - Single-temperature equation
 - Fixed boundary
 - Constant injection of neutrals in Gaussian centered on-axis

Quantitative agreement found in

- OD time histories
- 2D contours
 - Temperature
 - Current



M3D-C1 and NIMROD Coupling to KPRAD Successfully Benchmarked in Axisymmetric Simulations¹

- Both codes solved same problem of impurity injection into DIII-D core
 - DIII-D shot 137611 @ 1950 ms
 - 2D, nonlinear, single-fluid
 - Single-temperature equation
 - Fixed boundary
 - Constant injection of neutrals in Gaussian centered on-axis

Quantitative agreement found in

- 0D time histories
- 2D contours
 - Temperature
 - Current





M3D-C1 and NIMROD Coupling to KPRAD Successfully Benchmarked in Axisymmetric Simulations¹

- Both codes solved same problem of impurity injection into DIII-D core
 - DIII-D shot 137611 @ 1950 ms
 - 2D, nonlinear, single-fluid
 - Single-temperature equation
 - Fixed boundary
 - Constant injection of neutrals in Gaussian centered on-axis

Quantitative agreement found in

- OD time histories
- 2D contours
 - Temperature
 - Current



M3D-C1 Benchmark Run with Low-Resistivity Wall does not Qualitatively Change Results

- Results quantitatively match until contact with wall is made
- Current sheet opens and makes circuit with wall, before decaying away



M3D-C1 Benchmark Run with Low-Resistivity Wall does not Qualitatively Change Results

- Results quantitatively match until contact with wall is made
- Current sheet opens and makes circuit with wall, before decaying away



TOMICS



3D M3D-C1 Modeling Shows Stable Thermal Quench, Instability-Induced Current Quench with Ip Spike

- 3D, nonlinear simulation performed with M3D-C1 using argon benchmark initial conditions
 - 3D run is linearly stable throughout thermal quench due to axisymmetric deposition
 - Plasma sheet goes unstable, quenching current
- Instabilities cause current • to spike
 - Axisymmetric current
 - First spike of this magnitude in 3D MHD



3D Modeling Shows Stable Thermal Quench, Followed by Instability-Induced Current Quench with Ip Spike

- 3D, nonlinear simulation performed with M3D-C1 using argon benchmark initial conditions
 - 3D run is linearly stable throughout thermal quench due to axisymmetric deposition
 - Plasma sheet goes unstable, quenching current
- Instabilities cause curren to spike
 - Axisymmetric current
 - First spike of this magnitude in 3D MHD



3D Modeling Shows Stable Thermal Quench, Followed by Instability-Induced Current Quench with Ip Spike

- 3D, nonlinear simulation performed with M3D-C1 using argon benchmark initial conditions
 - 3D run is linearly stable throughout thermal quench due to axisymmetric deposition
 - Plasma sheet goes unstable, quenching current
- Instabilities cause current • to spike
 - Axisymmetric current broadens significantly
 - First spike of this magnitude in 3D MHD simulation



Lvons CTTS 4-19

Radial Localization Demonstrates 3D Mixing

- Same total number of particles injected in broad/narrow profile
- 2D: narrow has slower thermal quench
- 3D: mixing speeds up narrowdeposition thermal quench





Toroidally Localized Deposition Causes Early, Localized Instabilities

- Physical instabilities but eventually result in numerical crash
- Requires increasing resolution or diffusivities



Ongoing/Future M3D-C1 Work

- Complete 3D benchmark with NIMROD in near-term
- M3D-C1 pellet model extended allowing for multiple sources
 - SPI fragments
 - Multiple toroidal injection
- Focusing on simulations of toroidal localization of impurities
 - Eventually utilize toroidal-packing capability
 - Explore impact of extended deposition in toroidal angle
 - Allow for multiple toroidal injections (high-priority for ITER)
- Couple to Lagrangian-particle pellet-ablation code
- Validate simulations against experiments
 - DIII-D in near-term
 - KSTAR and JET in later years
- Predictive modeling for ITER



Pellet Ablation Studies in NIMROD C.C. Kim, J. McClenaghan



- Many small fragments increases ablation rate compared to monolithic pellet in same space
- Increased spreading of fragments over 1 ms plume decreases ablation (purple to red)
- Increasing plume length reduces ablation (blue to purple to red)
- Increasing isotropic viscosity above 10³ m²/s effects results
 - Despite no early MHD
 - Possibly decreases spreading, increasing shielding
- Details all result in minor variation in thermal quench time
 - δτ^{TQ} ~ 0.1 ms
 - Plume detail cause time offset but not diverging behavior



- Many small fragments increases ablation rate compared to monolithic pellet in same space
- Increased spreading of fragments over 1 ms plume decreases ablation (purple to red)
- Increasing plume length reduces ablation (blue to purple to red)
- Increasing isotropic viscosity above 10³ m²/s effects results
 - Despite no early MHD
 - Possibly decreases spreading, increasing shielding
- Details all result in minor variation in thermal quench time
 - $\delta \tau^{TQ} \sim 0.1 \text{ ms}$
 - Plume detail cause time offset but not diverging behavior



- Many small fragments increases ablation rate compared to monolithic pellet in same space
- Increased spreading of fragments over 1 ms plume decreases ablation (purple to red)
- Increasing plume length reduces ablation (blue to purple to red)
- Increasing isotropic viscosity above 10³ m²/s effects results
 - Despite no early MHD
 - Possibly decreases spreading, increasing shielding
- Details all result in minor variation in thermal quench time
 - δτ^{TQ} ~ 0.1 ms
 - Plume detail cause time offset but not diverging behavior



- Many small fragments increases ablation rate compared to monolithic pellet in same space
- Increased spreading of fragments over 1 ms plume decreases ablation (purple to red)
- Increasing plume length reduces ablation (blue to purple to red)
- Increasing isotropic viscosity above 10³ m²/s effects results
 - Despite no early MHD
 - Possibly decreases spreading, increasing shielding
- Details all result in minor variation in thermal quench time
 - $\delta \tau^{TQ} \sim 0.1 \text{ ms}$
 - Plume detail cause time offset but not diverging behavior



- Many small fragments increases ablation rate compared to monolithic pellet in same space
- Increased spreading of fragments over 1 ms plume decreases ablation (purple to red)
- Increasing plume length reduces ablation (blue to purple to red)
- Increasing isotropic viscosity above 10³ m²/s effects results
 - Despite no early MHD
 - Possibly decreases spreading, increasing shielding
- Details all result in minor variation in thermal quench time
 - $\delta \tau^{TQ} \sim 0.1 \text{ ms}$
 - Plume detail cause time offset but not diverging behavior



- Many small fragments increases ablation rate compared to monolithic pellet in same space
- Increased spreading of fragments over 1 ms plume decreases ablation (purple to red)
- Increasing plume length reduces ablation (blue to purple to red)
- Increasing isotropic viscosity above 10³ m²/s effects results
 - Despite no early MHD
 - Possibly decreases spreading, increasing shielding
- Details all result in minor variation in thermal quench time
 - $\delta \tau^{TQ} \sim 0.1 \text{ ms}$
 - Plume detail cause time offset but not diverging behavior



NIMROD SPI Simulations are Progressing - Kim

- Resistivity matched to experiment: η = 270.0 m²/s (@ 1eV), η_{min} = 0.1 m²/s (~ 200 eV)
- Simulations terminating due to high-n edge modes (RBM?)
 - High viscosity not sufficient
 - Tried Chodura resistivity but not sufficient
 - Hyper-resistivity reduces iterations but still crashes
 - Trying 3D thermal conduction
 - Okay for constant κ

• Can limit edge mode growth rate by using lower $\eta_{max} = 10 \text{ m}^2/\text{s}$ (~10eV)

- Limits Ohmic heating too much?
- Enough for RE acceleration and current quench?
- Maybe good enough (10eV is pretty cold for a thermonuclear plasma)
- Could go unstable later, maybe a particular solution for particular equilibrium
- High-n modes triggered by core tearing mode (2,1) and/or (3,2)?
 - reduce core resistivity (lower $\eta_{\text{min}})$ to reduce trigger ?



NIMROD Pellet Ablation Implementation Verified with PAM Code - McClenaghan

- Pellet ablation module (PAM) calculates pellet fueling deposition for transport studies
 - Fixed n_e and T_e
 - Calculates the same equations as NIMROD
- Benchmark setup
 - Pure deuterium pellet
 - Outboard-midplane launch
 - $r_p = 0.2 \text{ cm}, v_p = 500 \text{ m/s}$
- Good agreement between PAM and NIMROD when pellet is not deposited into the plasma
- Ablation changes when pellet is deposited into plasma
 - Currently under investigation





Steady-State Ablation and FronTier P.B. Parks



FronTier Model does not Permit Steady-State Ablation

- FronTier assumes a constant magnetic field and open (vacuum) boundary conditions in cylindrical system
- Lack of diamagnetism and background pressure, along with density-dependent diffusivity, result in constantly evolving radial ablation cloud
- Density-dependent diffusivity also requires infinitely opaque cloud in steady-state
- Reduced model captures these effects
- Steady-state would require finite background pressure, together with diamagnetic and magnetc tension forces



Mass Density in Ablation Channel is Determined by a Convection-Diffusion Equation

Mass transport:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_z}{\partial z} + \frac{1}{r} \frac{\partial}{\partial r} (r \rho u_r) = 0$$

- In low- β , far-field region (away from pellet)
 - Force-balance with deeply subsonic radial flows

$$\frac{\partial p}{\partial r} = J_{\theta} B$$

Ohm's Law

$$\eta_{\perp}J_{\theta} = -u_r B$$

Mass advects along and diffuses across field lines

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_z}{\partial z} = \frac{1}{B^2 r} \frac{\partial}{\partial r} \left(r \eta_\perp \rho \frac{\partial p}{\partial r} \right)$$

• or, if T is constant, $\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_z}{\partial z} = \frac{1}{r} \frac{\partial}{\partial r} \left(r \mathbf{D}_{\perp} \frac{\partial \rho}{\partial r} \right)$

$$\mathbf{D}_{\perp} = \frac{\eta_{\perp}p}{B^2}$$



Finite Pressure Gradient Continuously Expands into Vacuum Region – No Steady-State

- Pressure profiles in FronTier and reduced model have similar global structure
- Boundary of channel moves
 deeper into vacuum region
- Steady-state would require
 - Finite background pressure to raise diffusion
 - Diamagnetic currents to support pressure step at boundary



Finite Pressure Gradient Continuously Expands into Vacuum Region – No Steady-State

- Pressure profiles in FronTier and reduced model have similar global structure
- Boundary of channel moves deeper into vacuum region
- Steady-state would require
 - Finite background pressure to raise diffusion
 - Diamagnetic currents to support pressure step at boundary





Model Also Results in Infinite Opacity

- Finite opacity required or no heat flux to pellet (no abalation)
 - $\tau_{axis} = \int_{z_s}^{\infty} \rho dz \neq \infty$
 - Density ρ must fall off faster than 1/z for large z
- Reduced model gives logarithmic divergence in opacity
 - True even with u_z linearly increasing with z
 - More optimistic assumption than sublinear profile found in Frontier
- Not enough diffusion in far-field to allow for finite opacity
- Requires other means to make finite-length ablation cloud
 - Moving pellet
 - Curvature drift



Acknowledgments

- This work supported in part by US DOE contracts
 - DE-FG02-95ER54309,
 - DE-FC02-04ER54698,
 - and SciDAC CTTS (DE-SC0018109).
- This research used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S.
 Department of Energy Office of Science User Facility operated under Contract No. DE-AC02- 05CH11231.



Additional Slides



Higher resistivity allows must faster vertical displacement

- Future work
 - Optimal mesh to resolve wall contact
 - Match experimental L/R wall time



• Frontier is a time-dependent simulation of pellet ablation in a stationary B field surrounded by vacuo (Open Boundary Conditions)

• We developed a reduced model that shows no steady state is possible when a magnetized resistive medium (pellet cloud) expands into a vacuum

• We proved that stationary radial confinement of cloud is only possible when our resistive medium is surrounded by an ideal medium (hot plasma). Cloud is radially confined by diamagnetic surface current layer

• Our Convection diffusion model proved that in steady state the opacity of the cloud along the **pellet shadow** has a logarithmic divergence which prevents steady ablation rate. Cloud length must be limited? How?

 3D effects necessary, e.g., pellet motion and Alfven wave damping, curvature drift drive (Parks 1992, 2000, 2005, Rozhansky 1994)



Axisymmetric Steady-State Momentum Transport

$$- z \text{ component} \quad \rho \left(u_{z} \frac{\partial u_{z}}{\partial z} + u_{r} \frac{\partial u_{z}}{\partial r} \right) = -\frac{\partial p}{\partial z}$$
$$- r \text{ component} \quad \rho \left(u_{r} \frac{\partial u_{r}}{\partial r} + u_{z} \frac{\partial u_{r}}{\partial z} \right) = -\frac{\partial p}{\partial r} + J_{\theta} B$$
$$\frac{\partial \rho}{\partial r} = \frac{\partial \Gamma}{\partial r} + \frac{1}{2} \frac{\partial \rho}{\partial r} \left(-\frac{\partial \Gamma}{\partial r} \right) = -\frac{\partial p}{\partial r} + J_{\theta} B$$

- Mass Transport $\frac{\partial \rho}{\partial t} + \frac{\partial \Gamma_{\parallel}}{\partial z} = -\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \Gamma_{\perp}}{\partial r} \right) \qquad \begin{array}{c} \Gamma_{\parallel} = \rho u_z \\ \Gamma_{\perp} = \rho u_r \end{array}$
- In low- β far-field region the strong magnetic field inhibits radial flow
 - Ignore inertial terms in radial component of momentum equation

$$\rho\left(u_r\frac{\partial u_r}{\partial r} + u_r\frac{\partial u_r}{\partial z}\right) = -\frac{\partial p}{\partial r} + J_{\theta}B$$



In the Far-Field region of the Cloud the Radial flow Velocity is Diffusive like

 Cross-field Force balance

$$\frac{\partial p}{\partial r} = J_{\theta} B$$

- Ohm's law $\eta_{\perp} J_{\theta} = -u_r B$
- Eliminate current density J_{θ} to get radial flow

$$\longrightarrow$$
 $u_r = -\frac{\eta_\perp}{B^2} \frac{\partial p}{\partial r}$



Mass Density in Ablation Channel is determined by a Convection-Diffusion Equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_z}{\partial z} = \frac{1}{B^2 r} \frac{\partial}{\partial r} \left(r \eta_\perp \rho \frac{\partial p}{\partial r} \right) \qquad p = \frac{\rho}{m} (1 + Z)T \qquad \eta_\perp = \frac{m_e v_{ei}}{n_e e^2} = \frac{Z \ln \Lambda_{ei}}{9700 T (eV)^{3/2}}$$
(pressure)
(Spitzer cross-field
electrical resistivity)
$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_z}{\partial z} = \frac{1}{mB^2 r} \frac{\partial}{\partial r} \left\{ r \eta_\perp \rho \left[(1 + Z)T \frac{\partial \rho}{\partial r} + (1 + Z)\rho T \frac{\partial T}{\partial r} + \rho T \frac{\partial Z}{\partial r} \right] \right\}$$
- (large)
+ (small)
+ (small)
$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_z}{\partial z} = \frac{1}{r} \frac{\partial}{\partial r} \left(r D_\perp \frac{\partial \rho}{\partial r} \right) \qquad D_\perp = \frac{\eta_\perp p}{B^2} \qquad \text{classical cross-field}$$
Get same classical diffusion coefficient from the microscopic picture

$$D_{\perp} \sim \frac{(\text{electron gyro radius})^2}{\text{electron} - \text{ion collision time}}$$



FronTier Radial Pressure profiles has similar global structure as Parks' Reduced Model



• Radial flow velocity is zero when dp/dr = 0. But dp/dr = 0 when $p \sim 0$. in Frontier and in Parks model. That's a physical inconsistency! Cloud keeps expanding to find a new point where dp/dr = 0

ATOMICS

• Radial profiles at various times shows that the vr \propto dp/dr = 0 point keeps moving deeper and deeper into the vacuum region (no steady state)





• Attenuation of kinetic electron heat flux with increasing opacity



$$\tau(z) = \int_{z}^{\infty} \rho(r, z) dz$$

• The cloud "opacity" on axis must not diverge, otherwise the fast electrons would never reach the pellet and it would cease to ablate





Assume parallel flow velocity increases linearly with axial distance

$$U(z) \equiv \frac{u_z}{u_{z0}} = 1 + U' \cdot z$$

 $U' = \text{const velocity gradient} \lor$

• New Non-Linear equation in steady state becomes

$$(1+U'\cdot z)\frac{\partial\tilde{\rho}}{\partial z} = -\tilde{\rho} U' + \frac{1}{4r}\frac{\partial}{\partial r}\left(r\tilde{\rho}\frac{\partial\tilde{\rho}}{\partial r}\right)$$



The $\tilde{\rho}_{axis}$ tends to fall off faster with a Linearly increasing parallel velocity



• Opacity diverges logarithmically since the axial density profile falls off slower that 1/z

$$\tau_{axis} = \int_{z_s}^{\infty} \rho dz \quad ---> \quad \infty$$

