Calibrating mix models for NIF tuning

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Abstract. Mixing may play a role in early “tuning” implosions at the National Ignition Facility (NIF), intended for optimizing target geometry and laser operating parameters prior to the first ignition shots. Turbulent transport models allow mixing to be represented in integrated capsule-plus-hohlraum simulations, so that its effects can be predicted. Such models typically have many adjustable coefficients, so it is important to calibrate the coefficients systematically, whether by comparison to experiments, theory, or detailed higher fidelity simulations. We have begun by comparing to results from high-resolution 2D multimode simulations of a NIF Rev3 CH(Ge) ignition capsule, using the time-varying angle-averaged radial profiles of ion species composition as the calibration reference. 1D implosion simulations are performed with either of two turbulence models, and the models are calibrated so that the 1D composition profiles roughly match the 2D reference profiles at a sequence of five times near the end of the implosion. Details of the reference profiles, however, such as non-monotonicity resulting from structures in the flow, cannot be represented by these models. Parameter searches, besides identifying optimal sets of model coefficients, also exhibit model sensitivity to parameter variations.

1. Introduction
An imploding ICF capsule is subject to a variety of hydrodynamic instabilities resulting from strong gradients of density, pressure, and velocity in the converging flow [1]. The instabilities may amplify small perturbations in the flow field, leading to turbulence if the amplification proceeds far enough into the nonlinear regime. Nonlinear instability and turbulence in turn may drive “mixing”, i.e., the directed or diffusive interpenetration of ion species initially separated by a material interface (contact discontinuity). If instability, turbulence, and mixing arise in an implosion, they are expected to have a variety of deleterious effects on capsule behaviour. For example, in ignition capsules, early fine-scale instability and turbulence may lead to the break-up of the imploding shell. At later times, large-scale instability can deform the hotspot while fine-scale mixing contaminates the fuel. In implosion experiments performed during the tuning phase of NIF (prior to the first ignition tests), mixing can alter the size and shape of the imploded core of symmetry capsules, and change the areal density of the imploding capsule ablator. Thus, inferences about the adequacy of drive symmetry or the amount of unablated mass may be incorrect, if mixing is not accounted for.

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Given the importance of mixing and the potential severity of its effects, it is crucial to have a capability for representing it in numerical radiation–hydrodynamic simulations used for designing and analyzing future NIF implosions, to permit accounting for and mitigating its effects. The use of turbulent transport (“mix”) models to represent mixing in a NIF Rev3 CH(Ge) ignition capsule is described here. In particular, an approach for calibrating the coefficients in the models, the degree to which such models succeed in matching a reference simulation, and the sensitivity of model predictions to variations in the coefficients are discussed.

2. Numerical models of instability, turbulence, and mixing

The most widely accepted technique for credibly simulating the effects of instability, turbulence, and mixing in ICF capsules consists of high-resolution 2D and 3D nonlinear multimode simulations [2]. Such simulations, explicitly resolving spherical harmonic perturbation modes up to \( l = 1000 \) or higher, are computationally demanding and typically require representing the capsule alone (i.e., omitting the surrounding hohlraum). The effect of the hohlraum in creating a (possibly asymmetric) radiation drive is represented by a temporally and spectrally (and possibly angularly) varying radiation boundary condition on the capsule. This approach requires extracting the multidimensional radiation field information from a separate hohlraum calculation and mapping it to the nonlinear multimode simulation of the “stand-alone” capsule, a process that may introduce inaccuracies owing to phase-space averaging, inconsistent definition of boundaries, and the omission of hydrodynamic interactions between the hohlraum and capsule. While integrated (i.e., capsule plus hohlraum) simulations are certainly routine, to date they have not been used to resolve modes much above \( l = 12 \). It may be feasible to extend such simulations up to \( l = 30 \) or so, but high-resolution integrated simulations up to \( l \sim 1000 \) will not be feasible for the foreseeable future.

Given such limitations, it is worthwhile to consider turbulent transport (“mix”) models for representing mixing in integrated simulations. Such models introduce new field variables to describe the turbulent flow statistically, along with associated governing equations requiring simultaneous solution with the usual radiation–hydrodynamic equations. However, mix models typically have many adjustable coefficients and input parameters, so it is important to calibrate the coefficients systematically, with attention to the generality of and uncertainties in the result.

In the present study, a high-resolution 2D nonlinear multimode simulation of the type described in [2] has been used as a reference to calibrate two turbulent transport models: one developed by one of us (OS), which is referred to for brevity as the “Schilling K-\( \varepsilon \)” or “SK-\( \varepsilon \)” model, and one developed by Zhou, Zimmerman and Burke [3], which is referred to as the “ZZB” model. The SK-\( \varepsilon \) model uses two equations to describe the evolution of two quantities representing the turbulent field: \( K \), the turbulent kinetic energy density (with units \( L^2/T^2 \)) and \( \varepsilon \), the turbulent kinetic energy dissipation rate (with units \( L^2/T^3 \)). The modelled turbulent transport equations are

\[
\frac{\rho DK}{Dt} = -\frac{V_t}{\sigma_k} \frac{\nabla \rho}{\rho} \cdot \nabla p - \frac{\varepsilon}{\sigma_k} \frac{\nabla u - \rho \varepsilon}{\rho} + \nabla \left( \frac{\mu_k}{\sigma_k} \nabla K \right)
\]

\[
\frac{\rho D\varepsilon}{Dt} = -C_{e0} \frac{\varepsilon}{K} \frac{V_t}{\sigma_k} \frac{\nabla \rho}{\rho} \cdot \nabla p - C_{e1} \frac{\varepsilon}{K} \frac{\nabla u - C_{e2} \rho \varepsilon^2}{\rho} + \nabla \left( \frac{\mu_e}{\sigma_e} \nabla \varepsilon \right)
\]

where \( \rho \), \( p \), \( t \), and \( u \) denote density, pressure, time, and mean velocity, respectively, and \( D/Dt = \partial / \partial t + u \cdot \nabla \). These equations are coupled to the mean flow equations. The turbulent stress tensor is denoted by \( \tau \), the turbulent viscosity by \( \nu_t = \mu_t / \rho \), and the coefficients \( \sigma_k \), \( \sigma_e \), and \( \varepsilon \) (the turbulent Schmidt numbers) and \( C_{e0} \), \( C_{e1} \), and \( C_{e2} \) are to be calibrated. In the current study, a subset of these quantities was selected for calibration: the initial turbulent kinetic energy \( K_0 \) and turbulent length scale \( l_0 = K_0^{3/2}/\varepsilon_0 \) where \( \varepsilon_0 \) is the initial turbulent dissipation rate; multipliers \( M_{RT} \) and \( M_{RM} \) on the...
Rayleigh–Taylor part and the Richtmyer–Meshkov part, respectively, of the buoyancy production term, though they are usually constrained to be equal; and $\sigma_p$, $\sigma_z$, and $\sigma_d$, where $\sigma_p$ and $\sigma_z$ are always constrained to be equal. The four terms on the right-hand side of each equation represent buoyancy production of turbulence, shear and dilatation production, dissipation, and diffusive transport, respectively. In addition to these equations, there are other equations expressing the transport of each ion species by turbulent diffusion along a gradient.

ZZB is a two-scale turbulence model: it has equations for $K$ and $\epsilon$ similar to those in $SK\epsilon$, but the buoyancy production term is omitted. Instead, two additional equations are employed to represent the effect of buoyancy. One equation describes the buoyancy-drag velocity $V_i$:

$$\frac{dV_i}{dt} - \beta A g = -C_D \frac{\rho_i}{\rho_1 + \rho_2} \frac{V_i}{h_1},$$

where $A$ is the Atwood number, $g$ is acceleration, $\beta$ is a parameter, $C_D$ is the drag coefficient, and $h_1$ is the mixing layer width in region $i$, with $i = 1$ or 2 corresponding to light or heavy fluids, respectively.

The other equation is for the buoyancy energy $E_B$:

$$\frac{DE_B}{Dt} = S_B - \rho_B \nabla \cdot u - \frac{DE_B^{3/2}}{L_B} + \nabla \cdot (\rho \nabla \cdot E_B).$$

The dissipation rate of buoyancy energy (the third term on the right-hand side) appears as a source term in the $K$ equation. The two scales are a buoyancy length scale $L_B$, related to the mixing layer width, and a turbulent length scale $l = K^{3/2}/\epsilon$. The parameters used for calibration were the initial values $h_{10}$ and $h_{20}$ of the perturbation amplitude in the light and heavy fluids respectively, the time $t_{on}$ at which the model is turned on, and a multiplier $S$ on the turbulent diffusion coefficients.

3. Calibration

3.1. Calibration reference

Reduced-physics model coefficients can be calibrated via comparison to experiments, theory, or detailed higher fidelity simulations. As no actual ICF implosions conducted to date resemble pulse-shaped low-adiabat NIF implosions particularly well, a 2D multimode high-resolution simulation of a NIF ignition capsule has been used for calibration, especially because of the detailed temporal and spatial information that can be extracted from it. Here, the time-varying radial distribution of chemical composition in the imploding capsule predicted by the turbulence models is compared to the results from the high-resolution simulation. The simulation focused on a NIF Rev3 CH(Ge) ignition capsule, with outer radius 1.092 mm, a 165-µm-thick ablator with five layers of CH plastic doped with varying amounts of germanium (up to 0.6% by atom), a 75-µm-thick cryogenic DT fuel layer, and an inner DT vapour region with $\rho = 0.322$ mg/cm$^3$. The simulation was performed in a 9-degree sector, and an initial surface perturbation containing spherical harmonic modes $l = 40$-$1000$ was imposed on the fuel/ablator interface, with rms roughness 3.84 nm. The implosion was driven by a four-step Haan ignition pulse, input as a frequency-dependent radiation source whose equivalent temperature peaked at 310 eV at approximately 17 ns. Figure 1 (a) and (b) show radial profiles of the angle-averaged mass fraction of CH ablator extracted from this simulation at five times near the end of the implosion as open circles. The curves are labelled with their corresponding time, relative to an arbitrary reference: -600 ps, -400 ps, 0 ps, +400 ps, +800 ps. These curves constitute the calibration reference.

3.2. Calibration procedure and results

Numerous 1D simulations using either ZZB or $SK\epsilon$ were run, varying the model parameters and coefficients to achieve the closest possible match to the five reference profiles of Figure 1 at the corresponding times. This process was aided by scripts that varied the model inputs over desired ranges and automatically ran the simulations, and by use of a quantitative metric for goodness-of-fit (the average horizontal distance between the reference profile and the 1D model profile at each time).
Figure 1(a) shows a comparison of profiles of ablator mass fraction $f_{m,abl}$ from a 1D simulation using $SK$ to the reference profiles, with model parameters that give a reasonably good fit to the reference. Figure 1(b) shows a similar comparison for a 1D simulation using ZZB.

Figure 1. (a) Radial profiles of ablator mass fraction $f_{m,abl}$ plotted vs Lagrangian cumulative mass variable, at five times near the end of the implosion. Open circles show results from a high-resolution 2D multimode simulation [2]. The mixing front moves progressively inward to the left as time advances. Solid curves show results from a 1D simulation using $SK$ with $K_0 = 10^{-20}$ cm$^2$/ns$^2$, $l_0 = 10^{-5}$ cm, $MRT = MRM = 0.47$, $\sigma_p = 6.7$, and $\sigma_e = \sigma_c = 170$. (b) Same as (a), but solid curves show results from a 1D simulation using ZZB with $h_{10} = h_{20} = 2 \mu$m, $t_{on} = -530$ ps, and $S = 2$.

Figure 1 shows that both calibrated models agree reasonably well with the reference profiles, at all five times, for each profile’s “foot”, i.e., $1\% < f_{m,abl} < 20\%$. The agreement is not so good for smaller $f_{m,abl}$ (the “toe”, between 0.1\% and 1\%) or for larger $f_{m,abl}$ (the “plateau”, seen at $t = +800$ ps at $f_{m,abl} \sim 25\%$, and in the outward penetration of the mixing layer, at $f_{m,abl} > 30\%$). The discrepancies result to some extent from the definition of the goodness-of-fit metric, which focused on the foot. Other details of the reference profiles, such as the non-monotonicity seen at $t = -400$ ps at $f_{m,abl} \sim 0.2\%$, cannot be represented by the gradient-diffusion approximation for transport.

One result of the calibration exercise is the insight gained regarding the sensitivity of model predictions to variations in the inputs. For example, with the parameter settings used in Figure 1, variations of approximately $\pm 3\%$ in $\sigma_p$ in the $SK$ model lead to variations of approximately $\pm 5\%$ in the penetration of the mixing profile at $t = 800$ ps. The model is less sensitive to variations in $\sigma_e$ and $\sigma_c$; variations of $\pm 50\%$ in those coefficients give $\pm 5\%$ variation in the mixing penetration.

In future work, the predictive capability of the mix models will be assessed by calibrating against a similar implosion using a different initial perturbation. It is hoped that agreement with a reference can be achieved by varying only initial conditions, and not the model coefficients.

4. References
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