Project No. 09-791

Sharp Interface Tracking in Rotating Microflows of Solvent Extraction

Fuel Cycle R&D

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NEUP Nuclear Energy University Programs
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FINAL REPORT and QUARTERLY PROGRESS REPORT

Project Title: Sharp Interface Tracking in Rotating Microflows of Solvent Extraction

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Project Objective: The objective of this proposal is to develop a specialized sharp interface tracking simulation capability for predicting interaction of micron-sized drops and bubbles in rotating flows relevant to the understanding of contactor devices used in solvent extraction processes of nuclear spent fuel reprocessing. The primary outcome of this proposal is to determine from first principles the hydrodynamic mechanisms of mixing in a fluid contactor which enable rapid interfacial transport to occur in such a device. This result addresses the AFCI's technical work scope for CFD capabilities for process optimization. Our results uniquely support the AFCI vision of building novel levels of simulation for separations in both near and long terms. We developed algorithms for following the evolution of an organic/aqueous interface placed in a annular sector of a centrifugal contactor. The resulting simulation capability is aimed at predicting the evolution of a sharp interface under realistic fluid mixing conditions.

Status:

Overview. We have tested the developed simulation capability with the mixing of organic and aqueous phases in an annular sector representative of a commercial centrifugal contactor with a two-inch rotor diameter. The sector spans the entire gap of the mixing zone of the contactor while the axial and azimuth directions are truncated with periodic boundary conditions in the absence of gravity. The physical properties of the organic/aqueous system used in our numerical experiments were representative of a mixture of 30-vol% tri-*n*-butyl-phosphate in dodecane for the organic phase and a 1-M (molar) nitric acid solution for the aqueous phase. An initial volume of organic and aqueous phases is setup in the angular sector by means of a cylindrical interface shape. A volume fraction for the organic phase of about 0.45 was used. This is established by placing the aqueous phase on inner side of the cylindrical interface and the organic phase on the outer side. Given the aforementioned conditions and the assumption of incompressibility of both fluids, the volume fraction is an invariant of the underlying mathematical problem defined by the Navier-Stokes equations for both phases. Additional details of this computational procedure and model are described by Y. Zhou *et al.* 2012.

Our computational results for various angular sector sizes, mesh refinements and interfacial tension, indicate that the aqueous phase (heavier phase) evolves to the region near the outer radius of the annular gap. On the other hand, the organic phase (lighter phase)

evolves in the opposite direction. Therefore our calculations predict tremendous mixing by extensive stretching of the original interface and breakup resulting from the motion of the inner cylinder of the annular sector. As time evolves and the series of complex interface interactions take place the phases coalesce once more, but now at the correct position imposed by the centrifugal force. This regime is essentially a bicontinuous flow regime with relatively minor phase entrainment near the interface. A manuscript documenting these results, and further tests of the algorithms developed is in progress to be submitted for a peer review publication.

Issues not examined are the microstructure of the fluid flow at resolutions below current grid spacing (say $4\Delta x$ = 260 μm), and simulation time longer than 200 msec. Experimental observations of the microflow (de Almeida *et al* 2013) for the current system at similar values of the mixing parameters indicate that a dispersed phase always exists. Furthermore the organic phase tends to be the continuous phase for all values of the organic volume fraction about 0.5. While our computations could resolve drops of the dispersed phase at the average diameter value of 60 μm, it is the interstitial layer that challenges our computational limits. According to experiments, this layer is only a few micrometers thick at volume fractions near 0.5 and cannot be resolved with the current level of computational power available to us. Therefore the bicontinuous regime obtained in our simulations is a reasonable outcome for the current level of mesh refinement.

The time evolution of our simulations is about 200 ms using a rotor speed of 1500 rpm. Therefore it accounts for 5 revolutions of the rotor during the entire simulation. This evolution time is relatively short by comparison and will probably need to be increased in future studies. At the moment this simulation time is bounded by access to parallel computing power which is not easily available to us.

Statistical flow regimes. We have developed new theoretical and numerical approaches to the established study of turbulent mixing, as is described below. To assess the interfacial surface area, we have identified in part the statistically stationary flow regime for the mixing in an annular sector of a centrifugal contactor, in terms of the distribution of the fluid phases, statistically. There are three possible late time regimes, the first and second are stable two domain regimes with the heavy fluid (aqueous) dominantly on the outside and the light fluid (organic) on the inside. The third regime

is a chaotic mixture of droplets with length scales determined by the Weber number, *i.e.*, a few hundred micrometers. We call the first two regimes centrifuge modes, without wave breaking or with it and with resulting high levels of entrainment. Transitions to this statistical steady state are governed by Rayleigh-Taylor type instabilities. The third mode is a total entrainment mode, and the transitions to this mode are governed by the onset of Taylor-Couette flow. The choice among these three regimes depends on the device operation and fluid parameters.

We conduct simulations, which point to the two domain solution, with two dominantly single phase regions (by mass fraction), separated by a (wavy, unstable) interface, that is, regimes one and two. These simulations and the conclusion they reach are preliminary in the sense that larger simulation domain sizes may affect the stability of the various flow regimes; the three-phase flow with air may be a factor, and further simulation to late time may play a role. Current plans are to complete ongoing simulations to better assess the simulation domain size effect on the statistical steady flow regime observed.

In the first and second regime, with two separate phases (heavy outside and light inside), we identify turbulent diffusion as the primary hydrodynamic factor leading to rapid interfacial chemistry. In this regime we observe an increase of interfacial area of perhaps a factor of 10 relative to area of a simple cylindrical interface between the fluids, so that interfacial area plays a role in this regime also.

It is instructive to understand the evolution of the flow from a statistical perspective, especially as the information sheds light on the chemical reaction rates for interfacial chemical transport. We observe a transient chaotic stage to the flow, followed by a statistically stable flow configuration in regard to the bulk of the mass distribution. The stable flow has two distinct regions, with the light fluid (oil phase) on the inside and the heavy (aqueous) on the outside, and in each, a few droplets of the opposite phase. This statistically stable configuration has an augmented interfacial area relative to a simple cylindrical interface, but less than that observed during the transition to the steady state. The stable phases are formed by transit of droplets from their initial fluid location to the stable location. As we initialized the flow, the initial configuration is maximally unstable. The fluid is in the opposite location from the stable location, i.e. with the oil on the outside and the water on the inside. Experimentally, we expect a transition to a dispersion, in which interfacial area plays an important role.

We use a dispersion relation derived from Rayleigh-Taylor flow patterns and find the maximal unstable wave length to be in the range of 500 to 1000 microns, depending on the values assumed for the surface tension. A Weber number analysis predicts droplets of about 300 microns in size. This leads us to a mesh of no larger than 200 microns, although somewhat smaller meshes of 100 to 60 microns are needed and used for solution accuracy. We observe many small droplets, with more of them during the transient time regime, but their aggregate volume is not large. In the late time statistical steady state we observe a flow segregated into distinct domains, each with a dominant fluid by mass fraction.

Simulation studies of flow regimes. We pursued a number of simulations, to test the robustness of this picture. We vary the domain size, the physical parameters (surface tension), the numerical algorithm and the turbulence model. Further studies are in progress.

We initialize the flow in an unstable configuration, with all the light fluid (oil based) on the outside and all the heavy fluid (aqueous) on the inside. The interface between these fluids is unstable, and droplets of heavy and light fluid are formed. These migrate in their respective stable directions, namely the oil droplets to the inner radius and the water droplets to the outer radius. There, the droplets (which are quite numerous) coalesce, and form new continuous phases. The result is four continuous phases in layers, from the inside to the outside, as oil, water, oil, water. The two central phases and the interface between them are unstable. The unstable interface generates new unstable droplets, migrating to the two stable phases. In this manner, the two central phases disappear (due to losses from the droplet formation), leaving only the two stable phases as the statistical steady state, with a small number of droplets of the opposite phase embedded in each. We call this picture the centrifuge model of the steady state.

The theory of linear analysis can be applied to an interface located at a fixed radial value (a cylindrical interface). This interface is highly unstable, and we interpret the unstable modes as waves (as in waves on the ocean). As with the ocean waves, these waves can crest and lead to a new flow regime of entrainment flow, with two continuous phases (water outside, oil inside) but each with high levels of the other phase entrained as droplets inside it. Our simulations doe not decide between these two flow regimes, but we suspect that the preferred flow is a dispersion.

The determination of flow regime is the first step in developing an upscaled closure model of the flow. A manuscript documenting our conclusions is in preparation.

Time development of interface. In the figures below, we display the evolution of the fluid simulation.

Fig. 1 shows an early time unstable flow configuration, with the heavy fluid on the inside and the light fluid on the outside. Fig. 2 shows the interface between the two phases at a transient time. It has significant breakup of the simulation into droplets. In Fig. 3, we show by contrast a later time transitional flow, and in Fig. 4, a late time stable two-phase configuration.

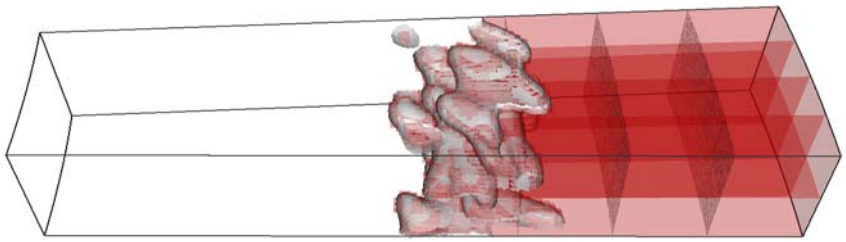

Fig. 1. Interface separating the two phases at an early time period.

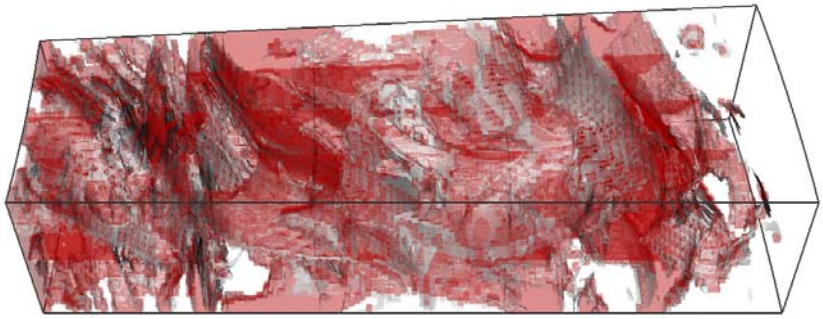

Fig 2. Interface separating the two phases at t = 161 ms.

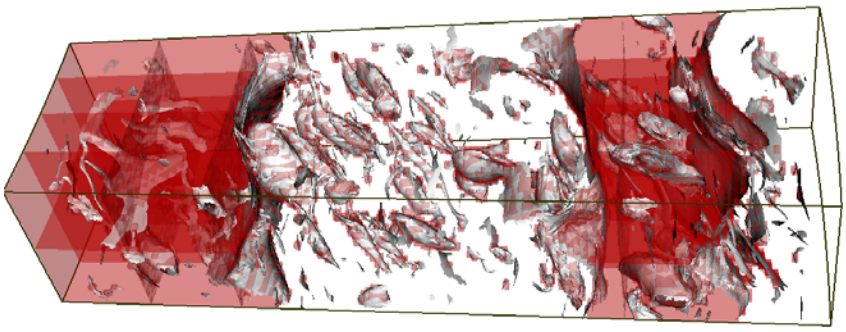

Fig. 3. At t = 240 ms, the two phase are now broken up into four domains, arranged from inner to outer radius, in which the dominant continuous phase is (in this order) light (oil, red), heavy, light (oil, red), and heavy.

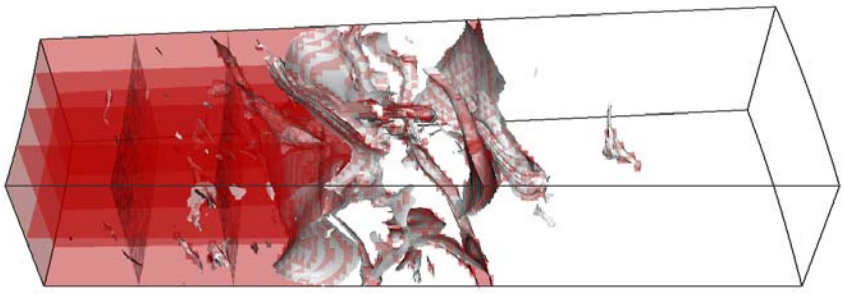

Fig. 4. At t = 475 ms, the fluids now lie in two domains, light on the inside and heavy on the outside.

Interfacial area and droplet size distribution. In this simulation, we analyze the interfacial area and the distribution of droplet sizes. The interfacial area is shown in Fig. 5. Observe the strong growth in area during the transient phase and the smaller level of interfacial area, still elevated relative to a simple cylindrical interface.

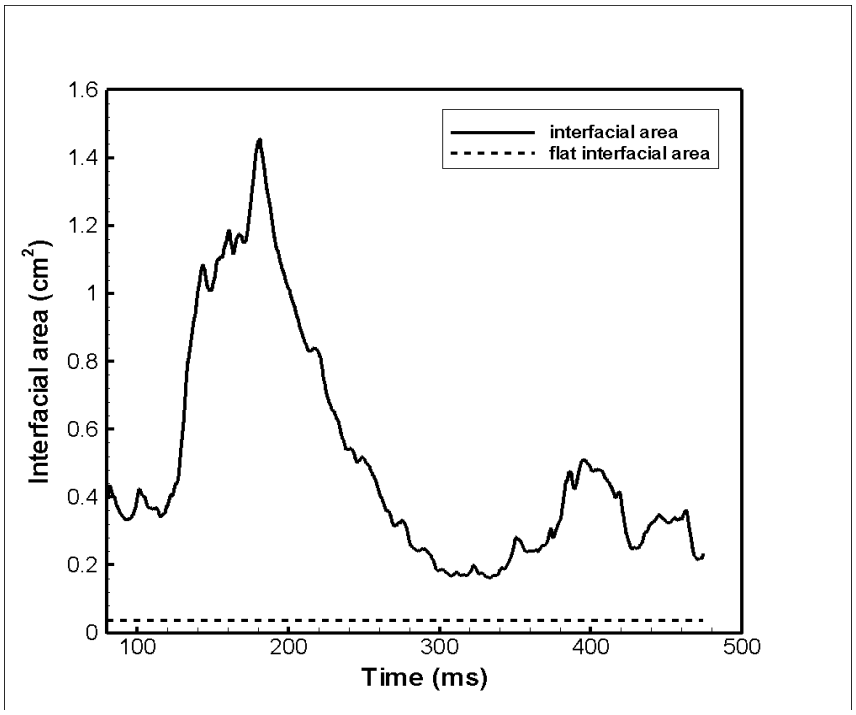

Fig. 5. Interfacial area clearly showing the transient and steady regimes with distinct patterns of interfacial area.

Fig. 6 shows the distribution of droplets, total volume vs. diameter and Fig. 7 shows the frequency vs. diameter. Both show the transient regime on the left and the late time on the right.

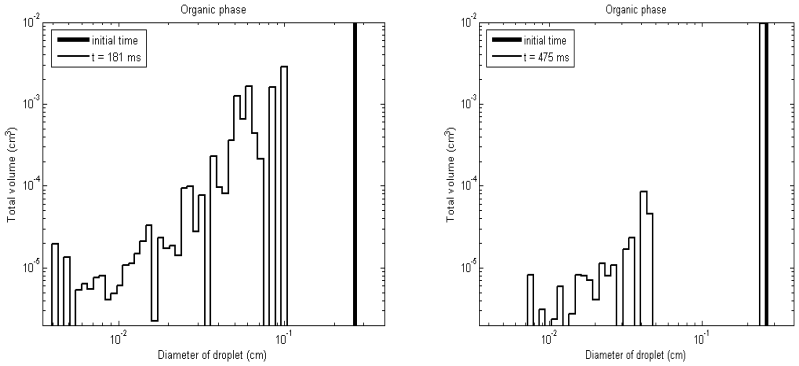

Fig. 6. Distribution of total droplet volume vs. diameter. Left: transient regime; right, late time.

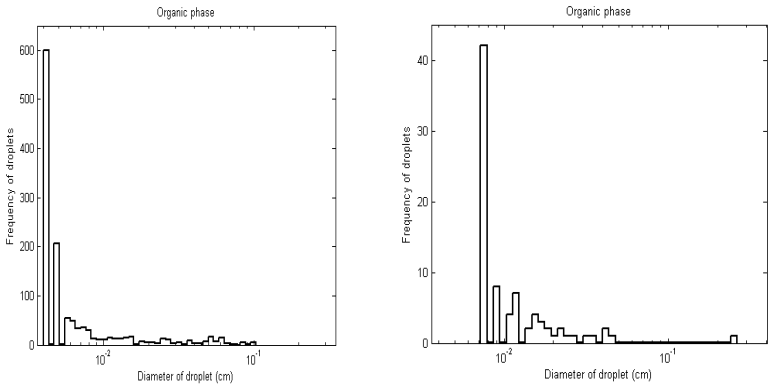

Fig. 7. Droplet distribution frequency vs. diameter. Left: transient right, late time. Note the change in vertical scales.

In all four frames, we observe a large number of small droplets, but the total volume occupied is small.

Turbulent diffusion. Chemistry, and distinct reacting species was out of the work scope of this project. Still, we can comment on the role of turbulent transport, known to be significant for diffusion limited reactions. Our analysis of the transport draws on analysis of other flows.

Chemical species in liquids diffuse relatively slowly, so that diffusion limited chemical reactions are common. Vigorous stirring leads to high Reynolds number flow and turbulence. At high Reynolds numbers, turbulent transport is usually more important than molecular transport. In Table 1, we list molecular and turbulent properties for the simulation considered here. The Schmidt number, the ratio of viscosity to species diffusion, is a dimensionless measure of species diffusion; it influences the rate of chemical reactions, especially diffusion limited ones. To assess turbulent diffusion, we examine a different (Rayleigh-Taylor) turbulent flow for the mixing of salt and fresh water at a common Reynolds number [Lim, Iwerks, Glimm and Sharp 2010]. See Table 1. Turbulent viscosity and turbulent species diffusion rates are mesh dependent, but in a recent study we observed quite stable values for their ratio, the turbulent Schmidt number, at high Reynolds numbers [Melvin, Rao, Kaufman, Lim, Yu, Glimm and Sharp 2012]. From Table 1, we conclude that turbulent viscosity plays a small role in our large eddy simulations (LES) of TC flow, but comparison to our RT flow suggests a strong role for turbulent diffusion, and the turbulent Schmidt number, once chemistry is considered, in addition to the hydrodynamics regime.

For chemically reacting flows, mixing at the atomic or molecular level is decisive, and thus the convergence of small scale fluctuations and not just mean values is important. We have begun a systematic study of convergence of solution fluctuations, based on the notion of w* convergence of a solution to a Young measure [Kamin, Kaufman, Glimm and Sharp 2012]. In this formulation, solution values are grouped into supercells, in a coarse graining that reduces the spatial resolution, but within each supercell, the ensemble of values is treated as a finite approximation to the fluctuating solution probability density function (PDF) of possible state values [Kaufman, Kamin, Yu and Glimm 2012], thereby enhancing the resolution of the statistical fluctuations. A tool to allow ready support for w* convergence studies is available.

http://www.ams.sunysb.edu/~rkaufman/api/

We obtain numerical evidence (verification) and some experimental confirmation (validation) for the convergence of fluctuation second moments and L_1 norm convergence of the cumulative distribution functions (CDFs) [Melvin, Rao, Kaufman and Glimm 2012, Lim, Yu, Glimm, Li and Sharp 2010].

	RT	TC (aqueous)	TC (organic)
Molecular visc.	1.0×10^{-2}	1.0×10^{-2}	1.9×10^{-2}
Turbulent visc.	8.0×10^{-4}	3.6×10^{-4}	2.3×10^{-4}
Molecular diff.	1.8×10^{-5}	--	--
Turbulent diff.	2.4×10^{-3}	--	--
Molecular Sc	5.6×10^{2}	--	--
Turbulent Sc	2.2×10^{-4}	--	--
Reynolds No.	2.5×10^{4}	2.5×10^{4}	12×10^{4}

Table 1. Viscosity (cm^2/s) and species diffusion (cm^2/s) for Rayleigh-Taylor and Taylor-Couette flows.

With the convergence of the full CDFs, we also obtain convergence of nonlinear functions of the flow field, such as reactive chemistry. We thus enable finite rate chemistry, in which the only chemical law added to the fluid flow is that of Arrhenius

chemistry. Omitted is a range of closure models otherwise needed to capture the internal structure of the chemical reaction; often such closure models are a prime source of solution uncertainty and error.

A path forward. Experiments by one of us (de Almeida *et al.*, 2013) suggest a picture for the late time flow, with many small droplets and a single continuous phase (a dispersion). We believe the primary difference of our simulations and the experimental results is due to the treatment of subgrid fluctuations, which in the present simulation call for merging of droplets when they come in contact, or even approach one another too closely. These merged droplets give rise to the two distinct continuous flow regimes we observe in the simulations. Here we propose a different subgrid scale picture, motivated by experimental high-speed imaging. If small droplets (60 microns, at a scale set by a Weber number) come in close contact, rather than merging, they may form a dispersion, and occupy the majority of the volume while still being a dispersed phase. Direct resolution of this phase will be difficult and perhaps unfeasible, but a subgrid model could be effective. In this model, droplets that come in contact would not merge, but retain a wall (double interface) between them, which will allow sliding, and whose forces would be modeled by appeal to lubrication theory. After obtaining agreement with experimental hydro quantities, we would consider chemistry and associated turbulent diffusion, as sketched below.

Molecular (Arrhenius) reaction rates. Observed bulk reaction rates are macroscopic and combine microscopic reaction rates with hydro issues. Here we indicate a route that in principle allows to connect these two reaction rates and predict either from a knowledge of the other. With W* convergence, for an LES simulation, we expect convergence for reactive chemistry as well. The hydro simulations, especially if developed further, will assess available surface area, while turbulent transport (turbulent species diffusion) will come from use of validated SGS models. Thus in principle, the hydro simulation code offers the possibility of a link between the chemical reaction rates as measured at these two different length scales.

Simulation code. We improved the existing simulation code through systematic upgrades of selected components. In remeshing, to ensure uniform surface triangles, we are now inserting new interface points using a higher order description of the interface. We have improved the algorithm, which calculates the phase volume of each phase. A systematic upgrade of the interface

algorithm to second and higher order accurate is partially completed.

We have developed a true second order accurate sharp interface algorithm, which is also robust for large density jumps, as occur at the air liquid interface. This code, once fully tested, will prove to be valuable to this area, as well as to the numerical community broadly speaking. Especially for large density contrasts, as with liquid air mixtures, this capability will be significant. Current tests indicate that the conservation properties of the current code will be sufficient for its intended application in the contactor problem.

We have improved the diagnostic capabilities, with an ability to track and diagnose individual droplets as they migrate from one flow region to another. The code has been transferred to ORNL and has been run from ORNL on INL hardware.

Extensive verification and some validation studies were conducted. The results of this effort were documented in a technical report, which has been published as an ORNL technical report (Y Zhou *et al* 2012). A new technical manuscript will be completed shortly, for journal submission.

Tasks:

Task 1: Preliminary 2D simulations

1. Task status: Completed. Lead investigators: J. Glimm and X. L Li.
2. Issues/Concerns: None
3. We are studying the extension of more accurate methods to the complete physics required.

Task 2: 3D simulations with realistic conditions

1. Task Status: Completed. Lead investigators: H. Lim, J. Glimm, X. Jiao, X. Li

2. Issues/Concerns: None.

Task 3: 2D/3D simulations with mesh refinement

1. Task Status: Completed; Lead investigator: James Glimm
2. Issues/Concerns: None

Task 4: Refined, verified solutions with publications

1. Task Status: We are formulating the contents of our first paper. Lead investigator: James Glimm
2. Issues/Concerns: We are completing a paper to describe the principle results of this project.

Patents/Publications:

T. Kaman, J. Glimm, and D. H. Sharp, Initial Conditions for Turbulent Mixing Simulations, Condensed Matter Physics, **13** (2010), 43401.

X. Jiao, D. Wang, and H. Zha, Simple and Effective Variational Optimization of Surface and Volume Triangulations, Engineering with Computers, 2010. DOI: 10.1007/s00366-010-0180-z.

Abstract: Optimizing surface and volume triangulations is critical for many advanced numerical simulation applications. We present a variational approach for smoothing triangulated surface and volume meshes to improve their overall mesh qualities. Our method seeks to reduce the discrepancies between the actual elements and ideal reference elements by minimizing two energy functions based on conformal and isometric mappings. We derive simple, closed-form formulas for the values, gradients, and Hessians of these energy functions, which reveal important connections of our method with some well-known concepts and methods in mesh generation and surface parameterization. We then introduce a simple and efficient iterative algorithm for minimizing the energy functions, including a novel asynchronous step-size control scheme. We demonstrate the effectiveness of our method experimentally and compare it against Laplacian smoothing and some other mesh smoothing techniques.

H. Lim, J. Iwerks, Y. Yu, J. Glimm and D. H. Sharp, Verification and Validation for Turbulent Mixing, Physica Scripta, **T142** (2010), 014014.

Y. Zhou, N. Ray, H. Lim, S. Wang, V. F. de Almeida, J. Glimm, X.-L. Li, and X. Jiao, Development of a Front Tracking Method for Two-Phase Micromixing of Incompressible Viscous Fluids with Interfacial Tension in Solvent Extraction. ORNL Technical Report ORNL/TM-2012/28.

V. F. de Almeida, J. F. Birdwell, D. W. DePaoli, and C. Tsouris, Microflow Visualization of Tri-*n*-butyl-Phosphate/Dodecane and Nitric Acid in a Centrifugal Contactor: Flow Regimes and Hysteresis. ORNL Technical Report ORNL/TM-2013/3.

V. F. de Almeida, Microflow Visualization of Tri-n-butyl-Phosphate/Dodecane and Nitric Acid in a Centrifugal Contactor: Supplementary Media. ORNL Technical Report ORNL/TM-2013/2.

T. Kaman, H. Lim, Y. Yu, D. Wang, Y. Hu, J.-D. Kim, Y. Li, L. Wu, J. Glimm, X. Jiao, X.-L. Li, R. Samulyak "A Numerical Method for the Simulation of Turbulent Mixing and its Basis in Mathematical Theory", In: "Lecture Notes on Numerical Methods for Hyperbolic Equations: Short Course Book", CRC Press/Balkema London. 2011, pages 105-129.

Xiangmin Jiao and Duo Wang, Reconstructing High-Order Surfaces for Meshing, Engineering with Computers, accepted and available online. October 2011. DOI: 10.1007/s00366-011-0244-8.

Abstract: We consider the problem of reconstructing a high-order surface from a given surface mesh. This problem is important for many meshing operations, such as generating high-order finite elements, mesh refinement, mesh smoothing and mesh adaptation. We introduce two methods, called Weighted Averaging of Local Fittings (WALF) and Continuous Moving Frames CMF). These methods are both based on weighted least squares polynomial fittings and guarantee C0 continuity. Unlike existing methods for reconstructing surfaces, our methods are applicable to surface meshes composed of triangles and/or quadrilaterals, can achieve third- and even higher order accuracy, and have integrated treatments for sharp features. We present the theoretical framework of our methods, experimental comparisons against other methods, and its applications in a number of meshing operations.

Duo Wang, Xiangmin Jiao, and James Glimm, Modeling and Discretization of Membranes with Normal Pressure Induced by Membrane Energy, submitted to Journal of the Mechanics of Physics of Solids, January, 2012.

G. Q. Chen and J. Glimm, Kolmogorov's Theory of Turbulence and the Invisid Limit of the Navier-Stokes Equations in R^3, Commun. Math. Phys., 310 (2012), pp. 267-283.

H. Lim, T. Kaman, Y. Yu, V. Mahadeo, Y. Xu, H. Zhang, J. Glimm, S. Dutta, D. H. Sharp, and B. Plohr. A Mathematical Theory of LES Convergence. Acta Mathematica Scientia 32 (2012) pp. 237-258.

T. Kaman, R. Kaufman, J. Glimm, and D. H. Sharp. Uncertainty Quantification for Turbulent Mixing Flows. Uncertainty Quantification in Scientific Computing , IFIP Advances in Information and Communication Technology 377 (2012) pp. 212-225.

J. Glimm, D. H. Sharp, T. Kaman and H. Lim. New Directions for Rayleigh-Taylor Mixing. Philosophical Transactions of the Royal Society. In press. 2012.

T. Kaman, J. Melvin, P. Rao, R. Kaufman, H. Lim, Y. Yu, J. Glimm and D. H. Sharp. Recent progress in turbulent mixing. Physica Scripta 2012 In Press.

R. Kaufman, T. Kaman, Y. Yu, J. Glimm. Stochastic Convergence and the Software Tool W*. Proceedings book of International Conference in honor of Professor E. F. Toro, CRC, Taylor and Francis Group. 2012, In Press.

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Bryan Clark, Navamita Ray, Xiangmin Jiao, Surface Mesh Optimization, Adaption, and Untangling with High-Order Accuracy, 21st International Meshing Roundtable, October 2012.

Y. Li, I-Liang Chern, J.-D. Kim and X.-L. Li, Numerical Method of Fabric Dynamics Using Front Tracking and Spring Model, Communications in Computational Physics, 2012.

H. Lim, J. Iwerks, J. Glimm and D. H. Sharp,. Nonideal Rayleigh Taylor Mixing. PNAS 107 (2010), pp 12786-12792.

J.-D. Kim, Y. Li and X.-L. Li, Simulation of Parachute FSI Using the Front Tracking Method, Journal of Fluids and Structures, Accepted, 2012.

J. Melvin, P. Rao, R. Kaufman, H. Lim, Y. Yu, J. Glimm and D. H. Sharp, Atomic scale mixing for Inertial Confinement Fusion Associated Hydro Instabilities, High Energy Density Physics, submitted 2012.

R. Kaufman, T. Kaman, Y. Yu and J. Glimm, Stochastic convergence and the software tool W*. Proceeding book of international conference to honor Prof. E. F. Toro. CRC, Taylor and Francis Group. 2012, pp. 37-41.

H. Lim, Y. Yu, J. Glimm, X.-L. Li and D. H. Sharp, Subgrid models for mass and thermal diffusion in turbulent mixing. Physica Scripta T142 (2010) pp 014062.

Presentations:

October 6, 2009, "Computational Science at Stony Brook's Department of Applied Mathematics and Statistics", Lehigh University, Bethlehem PA (Presentation by James Glimm)

January 13, 2010. "Collaborations/Partnerships with Engineering/Physics at Applied Mathematics and Statistics, Stony Brook", Invited mini-symposium talk. Joint Mathematics Meetings, San Francisco CA.

February 3, 2010. "Mathematical and Numerical Principles for Turbulent Mixing", Mathematics Department Colloquium, University of Pennsylvania, PA.

March 8, 2010. "Numerical Methods for Sharp Interfaces with DOE Applications" Invited Seminar, Mathematics and Computer Science Division, ORNL. Knoxville TN.

March 20, 2010. "Numerical Methods for Sharp Interfaces and Fluid Mixing". Invited Plenary Address, Midwestern PDE Conference, Evanston IL

March 22, 2010. "Mathematical and Numerical Principles for Turbulent Mixing", CAMS Distinguished Lecture, Univ. Southern California, Los Angeles CA.

J. Glimm April 6, 2010 "V&V for Turbulent Mixing with DOE Applications", X-Division Computational Physics Colloquium", Los Alamos National Laboratory, Los Alamos MN.

Abstract:
Turbulent mixing is important to LANL applications for example in the context of ICF performance, and prediction of mix related degration of fusion efficiency. It is an important input to turbulent combustion and to energy transport in climate studies, as well as in chemical processing.

Rayleigh-Taylor instability, driven by a continuous acceleration of a perturbed density jump interface, has been a challenge for 50 years in terms of comparison of simulation to experiment. With the mixing bubble penetration distance h expressed as h = alphaAgt^2, the determination

of the constant alpha has been widely studied.

Here we challenge the conentional view that alpha is a universal quantity that can be determined from universal (scale invariant, self similar) physics. We show that in the context of 14 laboratory experiments, simulation agreement with experiment is possible. Moreover, the simulations have sufficient precision to distinguish between individual experiments. Sensitivity of alpha to numerical effects such as numerical mass diffusion, to physical effects such as the Schmidt and Grashov numbers, and to initial ocnditions, not only the long wave length perturbations, but several other aspects ofhe initial conditions are sen to play a role in determing alpha. Mathematically, the scale invariant equations (the Euler equations) have non unique solutions. Numerically nonunique solutions are reported, in a turbulent mixing context. It seems that a common approach to V&V has hit a no-go theorem.

Beyond alpha, which sets one boundary of the mixing layer, we also explore the statistics of the temperature and concentration within the mixing layer. We find mesh convergence for the associated joint probability density functions, and as a result for the probability density function for a chemical reaction rate. This in a separate 2D Richtmyer Meshkov study.

Our numerical methods feature front tracking as well as dynamic subgrid scale models to define a parameter free LES simulation.

Contributions of collaborators and co-authors is gratefully acknowledged

J. Glimm May 26, 2010. "Mathematical, Physical and Numerical Principles for Turbulent Mixing", Minisymposium lecture, AIMS Conference, Dresden Germany.

Abstract:

Numerical mass diffusion is a characteristic problem in most simulation codes. In fluid mixing flows, numerical mass diffusion has the effect of over regularizing the solution.

A number of startling conclusions have recently been observed. For a flow accelerated by multiple shock waves, we observe an interface occupying a constant fraction of the available mesh degrees of freedom. This result suggests (a) nonconvergence for the unregularized mathematical problem, (b) nonuniqueness of the limit if it exists, and (c) limiting solutions only in the very weak form of a space time dependent probability distribution.

The cure for this pathology is a regularized solution, in other words inclusion of all physical regularizing effects, such as viscosity and physical mass diffusion.

In other words, the amount of regularization of an unstable flow is of central importance. Too much regularization, with a numerical origin, is bad, and too little, with respect to the physics, is also bad.

At the level of numerical modeling, the implication from this insight is to compute solutions of the Navier-Stokes, not the Euler equations. In the language of computational physics, the ILES (Implicit Large Eddy Simulation) formulation, which omits regularization, is scientifically incorrect.

Resolution requirements for realistic problems make this solution impractical in most cases. Thus subgrid transport processes must be modeled, and for this we use dynamic models of the turbulence modeling community. In the process we combine ideas of the capturing community (sharp interfaces or numerically steep gradients) with conventionalturbulence models, usually applied to problems relatively smooth at a grid level. With use of Front Tracking, we improve on this combination by reduction of numerical mass diffusion. Thereby, numerically steep gradients These ideas are developed in the context of numerical solution of turbulent mixing problems, some of long standing and some with applications to chemical processing and to turbulent combustion.

J. Glimm May 31, 2010. "Mathematical, Physical and Numerical Principles for Turbulent

Mixing", Partial Differential Equations Seminar, Oxford University, Oxford England.

Abstract

Numerical approximation of fluid equations are reviewed. We identify numerical mass diffusion as a characteristic problem in most simulation codes. This fact is illustrated by an analysis of fluid mixinf flows. In these flows, numerical mass diffusion has the effect of over regularizing the solution. Simple mathematical theories explain this difficulty.

A number of startling conclusions have recently been observed, related to numerical mass diffusion. For a flow accelerated by multiple shock waves, we observe an interface between the two fluids proportional to Delta x^-1, that is occupying a constant fraction of the available mesh degrees of freedom. This result suggests

(a) nonconvergence for the unregularized mathematical problem or

(b) nonuniqueness of the limit if it exists, or

(c) limiting solutions only in the very weak form of a space time dependent probability distribution.

The cure for the pathology (a), (b) is a regularized solution, in other words inclusion of all physical regularizing effects, such as viscosity and physical mass diffusion. We do notregard (c) as a pathology, but an inherent feature of the equations.

In other words, the amount and type of regularization of an unstable flow is of central importance. Too much regularization, with a numerical origin, is bad, and too little, with respect to the physics, is also bad. For systems of equations, the balance of regularization between the distinct equations in the system is of central importance.

At the level of numerical modeling, the implication from this insight is to compute solutions of the Navier-Stokes, not the Euler equations. Resolution requirements for realistic problems make this solution impractical in most cases. Thus subgrid transport processes must be modeled, and for this we use dynamic models of the turbulence modeling community. In the process we combine and extend ideas of the capturing community (sharp interfaces or numerically steep gradients) with conventional turbulence models, usually applied to problems relatively smooth at a grid level.

The numerical strategy is verified with a careful study of a 2D Richtmyer-Meshkov unstable turbulent mixing problem. We obtain converged solutions for such molecular level mixing quantities as a chemical reaction rate. The strategy is validated (comparison to laboratory experiments) through the study of 3D Rayleigh-Taylor unstable flows. are achieved.

These ideas are developed in the context of numerical solution of turbulent mixing problems, some of long standing and some with applications to chemical processing and to turbulent combustion.

J Glimm June 16, 2010. "V&V/UQ for Turbulent Mixing", Invited Lecture, 5th International Conference on Numerical Modeling of Space Plasma Flows. San Diego, CA.

Abstract:
Turbulent mixing is important in the context of ICF performance, and prediction of mix related degration of fusion efficiency. It is an important input to turbulent combustion and to energy transport in climate studies, as well as in chemical processing.

Rayleigh-Taylor instability, driven by a continuous acceleration of a perturbed density jump interface, has been a challenge for 60 years in terms of comparison of simulation to experiment. With the mixing bubble penetration distance h expressed as h = alphaAgt^2, the determination of the constant alpha has been widely studied.

We have challenged the conentional view that alpha is a universal quantity that can be determined from universal (scale invariant, self similar) physics. We show that in the context of 14 laboratory experiments, simulation agreement with experiment is possible. Moreover, the simulations often have sufficient precision to distinguish between individual experiments. Sensitivity of alpha to numerical effects such as numerical mass diffusion, to physical effects such as the Schmidt and Grashov numbers, and to initial ocnditions, not only the long wave length perturbations, but several other aspects ofhe initial conditions are seen to play a role in determing alpha.

Mathematically, the scale invariant equations (the Euler equations) have non unique solutions. Numerically nonunique solutions are reported, in a turbulent mixing context. It seems that a common approach to V&V has hit a no-go theorem. The 14 experiments for our validation test include both cases with measured initial conditions and those with no such measurement. They include one experiment modeled successfully by others and 13 others. For the experiments without measured initial conditions, we propose a method to reconstruct the initial Fourier spectrum of the perturbation from experimentally measured values. The experimental data is inconsistent with a frequently postulated Fourier power law k^{-1/3} for the initial data.

Beyond alpha, which sets one boundary of the mixing layer, we also explore the statistics of the temperature and concentration within the mixing layer. We find mesh convergence for the associated joint probability density functions, and as a result for the probability density function for a chemical reaction rate. This in a separate 2D Richtmyer Meshkov study.

James Glimm October 20, 2010. "Turbulent Mixing for a Jet in Crossflow and Plans for Turbulent Combustion". Poster presentation at PSAAP project meeting. Stanford, CA. Our numerical methods feature front tracking as well as dynamic subgrid scale models to define a parameter free LES simulation.

Jmaes Glimm October 28. "A Computer Science Approach to Interface Dominated Fluid Problems". CMACS Project Conference. New York University, NY.
November 9, 2010. "Supercomputing Study of Photovoltaic Quantum Dots", Advanced Energy Technologies Conference, New York, NY.

James Glimm November 22, 2010. "One Mathematician>s View of the Growing Role of Mathematics across Science and Beyond". Stelson Lecture, Georgia Institute of Technology, Atlanta GA

James Glimm November 23, 2010. "Mathematical, Numerical, and Physical principles for Turbulent Mixing. "Mathematics Colloquium Lecture, Georgia Institute of Technology, Atlanta GA.

James Glimm, January 18, 2011. "Numerical Errors for Solutions of Partial Differential Equations", CMACS Conference Presentation, Lehman College, New York City, NY.

James Glimm, March 4, 2011. "UQ for Turbulent Mixing" Minisymposium Invited Presentation. SIAM CS&E Conference, Reno NV.

James Gllimm, March 24, 2011. "Two Phase flow and Applications to Chemical Processing" Minisymposium plenary invited talk, 16th International Conference on Finite

Elements in Flow Problems, Munich, Germany.

Xiangmin Jiao, March 1, 2011, “Accurate and Conservative Data Remapping,” SIAM CS&E Conference, Reno, NV.

Front Tracking and Fluid Structure Interactions, Jungdong Kim, Yan Li and Xiaolin Li, SIAM CSE, Reno Nevada, March 1, 2011

Front Tracking on precipitation and dissolution, Yijing Hu and Xiaolin Li, SIAM CSE, Reno, Nevada, March 2, 2011.

James Glimm. May 3, 2011. "Mathematical theories of existence for 3D conservation laws and the nature of convergence in the large eddy simulation regime" Invited talk, Conference on Nonlinear Evolution Equations, Ann Arbor, MI.

James Glimm. July 4, 2011. "A numerical method for the simulation of turbulent mixing and its basis in mathematical theory" Short Course for Numerical Methods for Hyperbolic Equations, Santiago de Compostela, Spain.

James Glimm. July 5, 2011. "Mathematical theories of existence for 3D conservation laws and the nature of convergence in the large eddy simulation regime" Invited Plenary Lecture, Numerical Methods for Hyperbolic Equations, Theory and Applications, Santiago do Compostela, Spain.

James Glimm. August 3, 2011. "Uncertainty Quantification for Turbulent Reacting Flows". Plenary Lecture. Uncertainty Quantification in Scientific Computation NIST, Boulder CO.

James Glimm. August 25, 2011. "LES for Turbulent Miing and Combustion" Invited lecture. Turbulent Mixing and Beyond. ICTP, Trieste, Italy.

James Glimm. September 12, 2001. "Computational tools for LES Turbulent Mixing and Combustion". Lect

Navamita Ray, Duo Wang, Xiangmin Jiao, and James Glimm, High order computation of surface integrals over discrete surfaces, July 2011, Vancouver, BC, Canada.

Abstract: Surface integration is a fundamental operation in numerical computations. Integration over discrete surfaces is typically only second-order accurate due to piecewise linear approximations of the surface or the integrand. We propose a method that can achieve higher order of accuracy for surface integration. The method uses stabilized least squares approximation for local polynomial fittings and a blending
procedure based on linear shape functions. Experimental results demonstrate up to sixth order accuracy with our method.

Xiangmin Jiao, Some Mathematical Issues at Interfaces in Multiphysics Coupling, ICiS Multiphysics Workshop, July 2011, Park City, UT.

Duo Wang and Xiangmin Jiao, Noise-Resistant, Feature-Preserving, High-Order Surface Reconstruction for Surface Meshes, October 2011, Orlando FL, 2011.

Abstract: We consider the problem of reconstructing a high-order surface from a given surface mesh. We introduce two methods, called Weighted Averaging of Local Fittings (WALF) and Continuous Moving Frames (CMF), both based on weighted least squares polynomial fittings and guarantee C0 continuity. Our methods are applicable to surface meshes composed of triangles and/or quadrilaterals, can achieve third- and even higher order accuracy, and have integrated treatments for sharp features.

Bryan Clark, Duo Wang and Xiangmin Jiao, A Semi-Implicit Method of Mean Curvature Flow, SIAM Conference on Geometric & Physical Modeling, October 2011, Orlando FL, 2011.

Abstract: We propose a new semi-implicit method for mean-curvature flow using a triangulated surface. For spatial discretization, our method computes curvatures using a weighted least-squares approximation. To address the stiffness of the differential equation, we propose a semi-implicit method that enhances the stability and allows for a substantial enlargement of the time step. We present experimental comparisons with other methods to demonstrate the accuracy and stability of our proposed method.

ure at International Workshop on Numerical Methods and Modeling for Compressible Multimaterial Flows and Mixing. Beijing, China.

James Glimm. September 14, 2011. "LES for Turbulent Mixing and Combustion: Verification, Validation and Uncertainty Quantification". Lecture at International Woprkshop on Numerical Methods and Modeling for Compressible Multimaterial Flows and Mixing. Beijing, China.

James Glimm, September 12, 2001. "Computational tools for LES Turbulent Mixing and Combustion". Lecture at International Workshop on Numerical Methods and Modeling for Compressible Multimaterial Flows and Mixing. Beijing, China.

James Glimm, October 18, 2011. "V&V for Turbulent Mixing and Combustion". Invited Lecture for International Conference on Verification and Validation in Computational Science, Notre Dame, South Bend IN.

James Glimm, October 25, 2011. "Turbulence and Applications" Seminar Presentation, Rensselaer Polytechnic Institute, Troy, NY.

Feb. 21, 2012. "Simulation of Microfluidics and Droplet Statistics in a Contactor", NEUP workshop presentation, Corvallis, OR.

March 7, 2012, "Stochastic Convergence and Multiphysics Coupling", Colloquium Lecture, Iowa State University, Department of Aeronautical Engineering, Ames IA.

July 2012, "Mixing at the macroscale and molecular level for RM and RT instabilities in the limit of high Reynolds numbers", Conference presentation, International Workshop on the Physics of Compressible Turbulent Mixing, Woburn, UK.

October 2012, "Turbulent Mixing and Turbulent Reactive Flows" Plenary Lecture, 9th Asian Computational Fluid Dynamics Conference, Nanjing China.

October 2012, Xiangmin Jiao, "High-Order and Robust Numerical Computations over Complex Geometries", at Sandia National Laboratories.

October 2012, Navamita Ray, "Surface Mesh Optimization, Adaption, and Untangling with High-Order Accuracy", at 21st International Meshing Roundtable.

Front tracking on Fabric Modeling and Application to Parachute Dynamics, Wuhan Institute of Physics, Chinese Academia Sinica, July 6, 2012.

Front Tracking and Application in Fluid Physics, Departmental Colloquium, Beijing Normal University, July 4, 2012.

Front Tracking on Fabric Modeling and Application to Parachute Dynamics, Departmental Colloquium, Shanghai Jiaotong University, July 3, 2012.

Lagrangian Front Tracking Method to Fluid Instability Problems, Department of Mathematics, National Taiwan University, Taipei, March 19, 2012.

A Spring Model and the ODE System for the Study of Fabric Surface and Its Application in Parachute Simulation, Xiaolin Li, Joung-Dong Kim, and Yan Li, Department of Mathematics, National Sun Yat-sen University, Kaohsiung, Taiwan, March 21, 2012.

Front Tracking Method and Applications to Fabric Modeling and Parachute Simulation, Xiaolin Li, Joung-Dong Kim, and Yan Li, Department of Mathematics, National Cheng Kung University, Tainan, Taiwan, March 22, 2012.

Front Tracking Method and Applications to Fabric Modeling and Parachute Simulation, Xiaolin Li, Yan Li, I-Liang Chern, Joung-Dong Kim, East Asia SIAM Conference, Taipei, June 25, 2012.

Milestone Status Table:

Milestone/Task Description	Planned Completion Date	Actual Completion Date	Percent Complete
A user-friendly simulation code for tracking micro-drops and bubbles in annular gaps of centrifugal contactors using the front tracking method.	Q3 2012		100%

Milestone/Task Description	Planned Completion Date	Actual Completion Date	Percent Complete
Benchmark test problems, and provide standardized	Q3 2012		100%

result outputs for post-processing

. Milestone/Task DescriptionPlanned Completion DateActual Completion DatePercent Complete

Analysis and reporting of the results in peer reviewed journal. Q3 2012 85%

. Milestone/Task DescriptionPlanned Completion DateActual Completion DatePercent Complete

Task 1: 2D simulation of two-phase flow in realistic parameter regimes. Q2 2010 Q2 2010100%

Milestone/Task DescriptionPlanned Completion DateActual Completion DatePercent Complete

Task 2: 3D simulations in realistic parameter regimes; comparison to experimental data. Q3 2010 Q3 2010 100%

Milestone/Task DescriptionPlanned Completion DateActual Completion DatePercent Complete

Task 3: Mesh refinement studies for 2 D and 3D simulations and other verification tests. Q3 2011 Q4 2011100%

Milestone/Task DescriptionPlanned Completion DateActual Completion DatePercent Complete

Task 4: Two and three phase simulations, with experimental validation. Submission of results to a peer reviewed journal. Benchmark test problems for use in averaged equation validation studies. Q3 2012 85%

Students:

Name, Citizenship
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