Implementation of an air-entrainment model in interFoam for the course CFD with OpenSource Software

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Air entrainment modelling

The aim of this tutorial is to show how a sub-grid model for predicting the amount of air entrainment in an air-water system can be implemented based on `interFoam`.

Air entrainment

When the turbulence is high enough in free-surface flow, air will be entrained in the water phase and transported with the water flow

When the grid is not fine enough

- the processes at the surface will not be captured
  $\Rightarrow$ amount of air in water phase underestimated

interFoam

- Solves a single set of mass- and momentum equations

$$\nabla \boldsymbol{U} = 0$$

$$\frac{\partial \rho \boldsymbol{U}}{\partial t} + \nabla \cdot (\rho \boldsymbol{U}\boldsymbol{U}) = -\nabla p^* + \mathbf{g} \cdot \mathbf{x} \nabla \rho + \nabla \cdot \boldsymbol{\tau} + \mathbf{f}$$

- interFoam uses a VOF method with a compression term to capture the interface

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \boldsymbol{U}) + \nabla \cdot [\boldsymbol{U}_r \alpha (1 - \alpha)] = 0$$

where $\boldsymbol{U}_r = \boldsymbol{U}_1 - \boldsymbol{U}_2$ is the relative velocity

The subgrid model

The implementation shown in this tutorial will represent a try on reproduce the model introduced in Flow-3D by Hirt (2003)

$$\frac{\delta V}{\delta t} = C_{air} A_s \sqrt{2 \frac{P_t - P_d}{\rho}}$$

$$P_t = \rho k$$

$$P_d = \rho g_n L_T + \frac{\sigma}{L_T}$$

$$L_T = C_\mu \sqrt{\frac{3}{2}} \frac{k^{3/2}}{\epsilon}$$

The subgrid model - requirements

Our air-entrainment model requires the knowledge of:

- where the surface is located
- the normal of the surface
- the surface tension
- turbulence variable (k and ϵ)
- Mesh properties

`interFoam` - *immiscibleIncompressibleTwoPhaseMixture*

Integration of subgrid model

```
class immiscibleIncompressibleTwoPhaseMixture
:
    public incompressibleTwoPhaseMixture,
    public interfaceProperties
```

Takes care of transport properties and interface properties

```
//- Correct the transport and interface properties
virtual void correct()
{
    incompressibleTwoPhaseMixture::correct();
    interfaceProperties::correct();
}
```

Integration of subgrid model

`interFoam` - *immiscibleIncompressibleTwoPhaseMixture*
$\Rightarrow$ `interAirEntFoam` - *airEntrainmentTwoPhaseMixture*

- And add calculation of the air entrainment model
- Implement functions for the model variables and ρ_{mix}

Variable	Function in airEntrainmentTwoPhasMixture
L_T	volScalarField Lt(k,ϵ)
P_t	volScalarField Pt(k)
P_d	volScalarField Pd(k,ϵ)
S_g	volScalarField calcSource(U,k,ϵ)
ρ_{mix}	void updateRhomix()

interFoam → interAirEntFoam

Adding

$$\frac{\delta V}{\delta t} = C_{air} A_s \sqrt{2 \frac{P_t - P_d}{\rho}}$$

As an explicit source term

$$\frac{\partial \alpha_l}{\partial t} + \nabla \cdot (\alpha_l \mathbf{u}) + \nabla \cdot [\mathbf{u}_c \alpha_l (1 - \alpha_l)] = S_g \quad (1)$$

where

$$S_g = \frac{\frac{\delta V}{\delta t}}{mesh.V()}$$

interFoam - solution algorithm

Basic structure of the solver

- Initiate fields
- Starting runtime loop
  - Calculating time step
  - Iterating over the PIMPLE Loop nOuterCorrectors times
    - Solving the α-equation (VOF and MULES)
    - Calculate the interface and transport properties
    - Solving the momentum equation
    - PISO Loop over pressure equation
  - Calculate the turbulent properties

interFoam → interAirEntFoam

This section will provide the steps in the implementation of the air entrainment model named, interAirEntFoam.

```
cd $WM_PROJECT_USER_DIR/
mkdir -p applications/solvers/multiphase/
cd !$
cp -r $FOAM_SOLVERS/multiphase/interFoam/ .
```

Rename the solver and the files to interAirEntFoam

```
mv interFoam interAirEntFoam
cd !$
mv interFoam.C interAirEntFoam.C
```

interFoam → interAirEntFoam

Remove folders not needed

```
rm -r interMixingFoam overInterDyMFoam
```

Rename within the files

```
sed -i s/interFoam/interAirEntFoam/g Make/files
sed -i s/interFoam/interAirEntFoam/g interAirEntFoam.C
```

Change the name of the excutable path

```
sed -i s/APPBIN/USER_APPBIN/g Make/files
```

Then you have to update the Make/options file, to include the desired libraries

```
EXE_INC = \
  -I$(FOAM_SOLVERS)/multiphase/VoF \
```

Copy immiscibleIncompressibleTwoPhaseMixture

Find the location of immiscibleIncompressibleTwoPhaseMixture and copy it to your folder

```
find $WM_PROJECT_DIR -name  immiscibleIncompressibleTwoPhaseMixture
cp -r $FOAM_SRC/transportModels/immiscibleIncompressibleTwoPhaseMixture .
```

Change the name of the model and its files

```
mv immiscibleIncompressibleTwoPhaseMixture airEntrainmentTwoPhaseMixture
cd airEntrainmentTwoPhaseMixture
mv immiscibleIncompressibleTwoPhaseMixture.C airEntrainmentTwoPhaseMixture.C
mv immiscibleIncompressibleTwoPhaseMixture.H airEntrainmentTwoPhaseMixture.H
sed -i s/immiscibleIncompressible/airEntrainment/g Make/*
sed -i s/immiscibleIncompressible/airEntrainment/g airEntrainmentTwoPhaseMixture.*
```

airEntrainmentTwoPhaseMixture

And rename in the solver to call the new library

```
cd ..
sed -i s/immiscibleIncompressible/airEntrainment/g createFields.H
sed -i s/immiscibleIncompressible/airEntrainment/g interAirEntFoam.C
```

At this point you have a local version of the `immiscibleIncompressibleTwoPhaseMixture` named `airEntrainmentTwoPhaseMixture`

$\Rightarrow$ Change the name of the library path in Make/files accordingly:

```
sed -i s/LIBBIN/USER_LIBBIN/g airEntrainmentTwoPhaseMixture/Make/files
```

airEntrainmentTwoPhaseMixture

Change relative paths in
airEntrainmentTwoPhaseMixture/Make/options

```
EXE_INC = \
    -I$(LIB_SRC)/transportModels \
    -I$(LIB_SRC)/transportModels/incompressible/lnInclude \
    -I$(LIB_SRC)/transportModels/interfaceProperties/lnInclude \
    -I$(LIB_SRC)/transportModels/twoPhaseMixture/lnInclude \
    -I$(LIB_SRC)/finiteVolume/lnInclude
```

Compile to check that it works

```
wmake airEntrainmentTwoPhaseMixture
```

Link to airEntrainmentTwoPhaseMixture

Now you want your new solver `interAirEntFoam` to use this library

$\Rightarrow$ link to it in the Make/options file within the solver as

```
-L$(FOAM_USER_LIBBIN) \
-lairEntrainmentTwoPhaseMixture
```

Link to the new directory has to be linked to under EXE_INC

```
-IairEntrainmentTwoPhaseMixture \
```

Make sure that the name written in the Make/options file corresponds to the library it is written to

Test the model

Compile it

```
wmake airEntrainmentTwoPhaseMixture
wmake
```

When both the library and the solver compiles, you should copy the damBreak tutorial, and run it with your new solver:

```
cp -r $FOAM_TUTORIAL/multiphase/interFoam/RAS/damBreak/damBreak $FOAM_RUN
run
cd damBreak
sed -i s/interFoam/interAirEntFoam/g system/controlDict
./Allrun
```

Ready to implement

The solver should return the output of the source term

$$\frac{\delta V}{\delta t} = C_{air} A_s \sqrt{2 \frac{P_t - P_d}{\rho}}$$

This term is a function of several terms, that we will calculate in separate member functions within the model

$$\frac{\delta V}{\delta t} = f(P_t(k, \rho), P_d(L_T, k, g, \epsilon), \rho, C_{air}, A_s)$$

The implementations are done in `airEntrainmentTwoPhaseMixture.H` and `airEntrainmentTwoPhaseMixture.C`

Calculation of P_t

Calculate a density for the mixture, we do this by introducing a private member variable in `airEntrainmentTwoPhaseMixture.H`

```
// Private data
volScalarField rhomix_;
```

that we initiate in the constructor (in `airEntrainmentTwoPhaseMixture.C`)

```
rhomix_
(
    min(max(alpha1(), scalar(0)), scalar(1))*rho1_ +
    (scalar(1) - min(max(alpha1(), scalar(0)), scalar(1)))*rho2_
)
```

Calculation of P_t

Create an update function to update the mixture density each time we call the source term from the solver, in the header file

```
void updateRhomix();
```

We implement the calculation of this function in .C-file

```
void Foam::airEntrainmentTwoPhaseMixture::updateRhomix()
{
  rhomix_ = min(max(alpha1(), scalar(0)), scalar(1))*rho1_
          +(scalar(1) - min(max(alpha1(), scalar(0)),scalar(1)))*rho2_;
}
```

Then we are ready to implement P_t

Calculation of P_t

We declare the function for the perturbating term P_t in the .H-file

```
// - Calculates the pertubing component that makes the flow unstable
// - and returnes a volumScalarField
volScalarField Pt(const volScalarField k);
```

and implement it in the .C-file

```
Foam::volScalarField Foam::airEntrainmentTwoPhaseMixture::Pt(const
                                                    volScalarField k)
{
    updateRhomix();
    volScalarField Pt = k*rhomix_;
    return Pt;
}
```

P_d, L_T, and calcSource are implemented in a similar manner

Calculation of L_T

We declare the function in the header file

```
// Calculates Lt (the characteristic turbulent length scale)
volScalarField Lt(
                  const volScalarField k,
                  const volScalarField epsilon
);
```

And implements the function in the .C-file

```
Foam::volScalarField Foam::airEntrainmentTwoPhaseMixture::Lt(
     const volScalarField k,
     const volScalarField epsilon)
{
    dimensionedScalar dimCorr("dimCorr",dimLength/dimTime,1);
    volScalarField newepsilon = epsilon +
      dimensionedScalar("smallEpsilon",dimensionSet(0,2,-3,0,0,0,0),1e-10);
    volScalarField Lt = 0.09*sqr(1.5)*pow(k,3/2)/newepsilon*dimCorr;
    return Lt;
}
```

Additional member variables

The calculation of P_d needs the surface tension and gravity

$$P_d = \rho g_n L_T + \frac{\sigma}{L_T}$$

The calculation of the source term needs C_{air}

$$\frac{\delta V}{\delta t} = C_{air} A_s \sqrt{2 \frac{P_t - P_d}{\rho}}$$

we add these variables as private member variables in our class

```
// Private data
    const dimensionedScalar sigma_;
    uniformDimensionedVectorField g_;
    const dimensionedScalar Cair_;
```

Here we introduce a new variable type
$\Rightarrow$

```
#include "uniformDimensionedFields.H"
```

Additional member variables

We initialize these member variables in the constructor accordingly

```
sigma_
(
    "sigma", dimensionSet(1,0,-2,0,0,0,0), lookup("sigma")
),
Cair_
(
    "Cair", dimensionSet(0,0,0,0,0,0,0), lookup("Cair")
),
g_(
    IOobject
    (
        "g",
        U.time().constant(),
        U.mesh(),
        IOobject::MUST_READ_IF_MODIFIED,
        IOobject::NO_WRITE
    )
)
```

These variables are read and changed from the input case files

Calculation of P_d

declare the function in the header file

```
// Calculates the stabilizing surface force Pd
volScalarField Pd(
        const volScalarField k,
const volScalarField epsilon
);
```

And implements the function in the .C-file

Calculation of P_d

```
Foam::volScalarField Foam::airEntrainmentTwoPhaseMixture::Pd(
                                                    const volScalarField k,
                                                    const volScalarField epsilon)
{
    // Calculate surface normal
        // Cell gradient of alpha
    const volVectorField gradAlpha(fvc::grad(alpha1(), "nHat"));
    // Unit interface normal
    volVectorField nHat(gradAlpha/(mag(gradAlpha) + deltaN()));
    // Gravitation forces normal to surface
    volScalarField gn = g_ & nHat;
    volScalarField lLt = Lt(k,epsilon);
    // Calculates the stabilizing surface force Pd
    updateRhomix();
    volScalarField Pd = rhomix_*mag(gn)*lLt + sigma_/lLt;
    return Pd;
}
```

Calculation of P_d

The implementation of P_d make use of the namespace `fvc`

$\Rightarrow$ Include the fvCFD.H in airEntrainmentTwoPhaseMixture.H

```
#include "fvCFD.H"
```

and link to meshTools in airEntrainmentTwoPhaseMixture/Make/options as

```
-I$(LIB_SRC)/meshTools/lnInclude \


-lmeshTools \
```

Calculation of S_g

Finally the source term S_g can be calculated as a volume fraction term

- We declare the function in the header file

```
//- Calculates source term, returned as volum fraction rate
volScalarField calcSource(
        const volVectorField& U,
        const volScalarField k,
        const volScalarField epsilon
);
```

And implement the function in the .C-file

Calculation of S_g

```
Foam::volScalarField Foam::airEntrainmentTwoPhaseMixture::calcSource(
     const volVectorField& U,
     const volScalarField k,
     const volScalarField epsilon)
{
    Info << "calcSource" << endl;

    // Initialize the volume fraction rate term, as 0 or 1 for on interface
    volScalarField dvdt(nearInterface());
    volScalarField Afs(dvdt);

    // Estimate cell surface area as V^(2/3)
    forAll(Afs, cellI)
    {
        Afs[cellI] = pow(U.mesh().V()[cellI],0.67);
    }

    volScalarField Pdl = Pd(k,epsilon);
    volScalarField Ptl = Pt(k);
    updateRhomix();
```

Calculation of S_g

```
    // Calculate the volume fraction rate term
    forAll(dvdt, cellI)
    {
     if((Ptl[cellI] > Pdl[cellI])){
         scalar air2cell = dvdt[cellI]*Cair_.value()*Afs[cellI]*
          sqr(2*(Ptl[cellI]-Pdl[cellI])/rhomix_[cellI])
          /U.mesh().V()[cellI];
         dvdt[cellI] = -min(air2cell,0.5);
     }else{
         dvdt[cellI] = scalar(0.0);
     }
    }

    forAll(dvdt.boundaryField(), patchI)
    {
forAll(dvdt.boundaryField()[patchI], faceI )
{
    dvdt.boundaryFieldRef()[patchI][faceI] = scalar(0.0);
}
    }

    dimensionedScalar dimCorr("dimCorr",dimVelocity/dimLength,1);

    return dvdt*dimCorr;
}
```

Add source term to α_l-equation

Add source term to the α_l-equation as the explixit source term S_u in `alphaSuSp.H`. Creates this field in `createFields.H`

```
// Source term for visualization
volScalarField Su
(
    IOobject
    (
        "Su",
        runTime.timeName(),
        mesh,
        IOobject::READ_IF_PRESENT, //NO_READ,
        IOobject::AUTO_WRITE //NO_WRITE
    ),
    mesh,
    dimensionedScalar("Su",dimVelocity/dimLength, 0)

);
```

Let it be updated for every time step by adding a call to `calcSource` from `alphaSuSp.H`

```
Su = mixture.calcSource(U,turbulence->k(),turbulence->epsilon());
```

Add source term to α_l-equation

The solution algorithm in `alphaEqn.H` solves Equation (1) successively using MULES compression. This results in a limited flux:

$$\phi_{\alpha,l} = \phi_{\alpha,l}^{UD} + \phi_{\alpha,l}^{lim,Corr}$$

where

$$\phi_{\alpha,l}^{lim,Corr} = \theta_l \cdot \phi_{\alpha,l}^{Corr} = \theta_l \cdot (\phi_{\alpha,l}^{HO} + \phi_{\alpha,l}^{C} - \phi_{\alpha,l}^{UD})$$

The MULES compression, that are included to make the interface sharp, is possible to turn off by the user by setting the user parameters accordingly (`MULESCorr` to `false` and `cAlpha` to 0). Then the flux is calculated to be

$$\phi_{\alpha,l} = \phi_{\alpha,l}^{HO}$$

which means that only the higher order fluxes, using the discretization scheme given for `div(phi,alpha)` in `divSchemes` in the `system/fvSchemes` input file, is used for calculating the fluxes of α_l.
If `MULESCorr` is set to `false` and `cAlpha` $\neq 0$, then $\phi_{\alpha,l}$ is calculated as:

$$\phi_{\alpha,l} = \theta_l \cdot (\phi_{\alpha,l}^{HO} + \phi_{\alpha,l}^{C})$$

Add source term to α_l-equation

S_u added in the calculation of the upwind flux if MULES is activated

```
if (MULESCorr)
{
    #include "alphaSuSp.H"

    fvScalarMatrix alpha1Eqn
    (
        (
            LTS
          ? fv::localEulerDdtScheme<scalar>(mesh).fvmDdt(alpha1)
          : fv::EulerDdtScheme<scalar>(mesh).fvmDdt(alpha1)
        )
      + fv::gaussConvectionScheme<scalar>
        (
            mesh,
            phiCN,
            upwind<scalar>(mesh, phiCN)
        ).fvmDiv(phiCN, alpha1)
    // - fvm::Sp(fvc::ddt(dimensionedScalar("1", dimless, 1), mesh)
    //           + fvc::div(phiCN), alpha1)
      ==
        Su + fvm::Sp(Sp + divU, alpha1)
    );

    alpha1Eqn.solve();
```

Add source term to α_l-equation

If MULES = `false`, S_u to added in MULES::explicitSolve

```
MULES::explicitSolve
(
    geometricOneField(),
    alpha1,
    phiCN,
    alphaPhi10,
    Sp,
    (Su + divU*min(alpha1(), scalar(1)))(),
    1,
    0
);
```

Vertical plunging jet

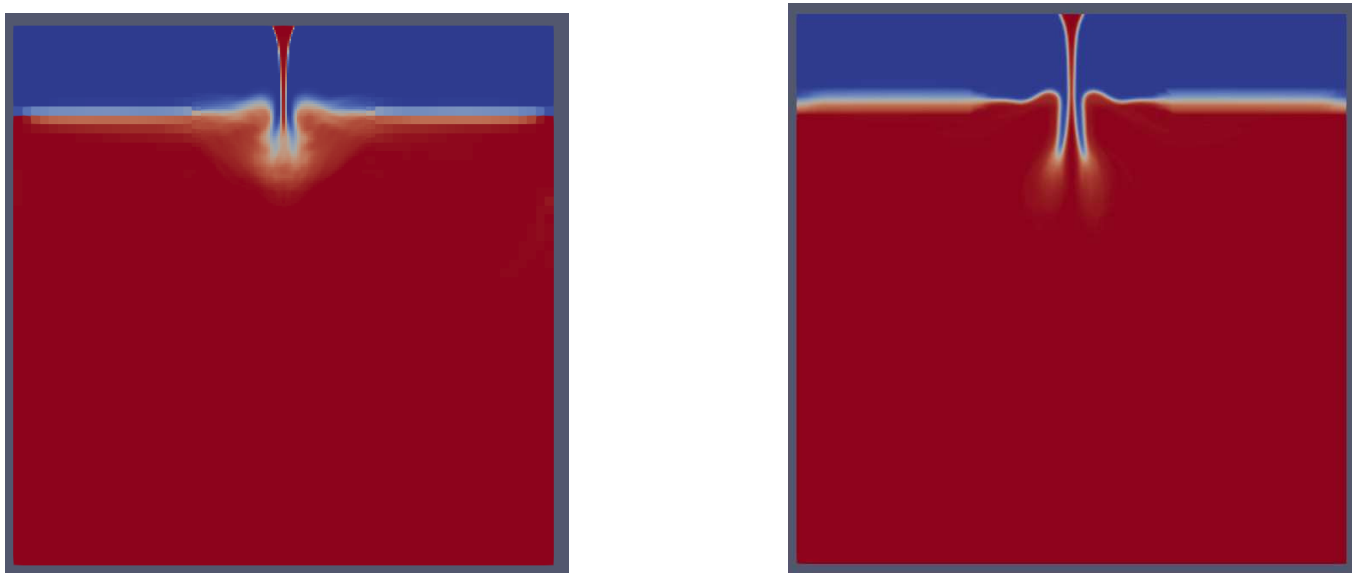
Download the test case to your user directory. Then go into the case directory and run the Allrun-script

```
cd $FOAM_RUN/jetIntoPool
./Allrun &
```

Then copy the case, to a new folder, and run it with `interFoam` to compare the behavior

```
cd ..
cp -r jetintopool jetintopool_interFoam
sed -i s/interAirEntFoam/interFoam/g system/controlDict
./Allrun &
```

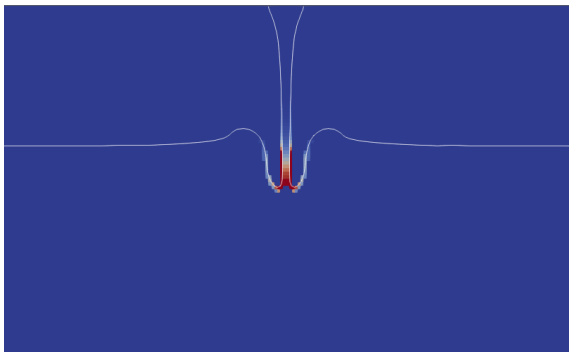
Vertical plunging jet – results



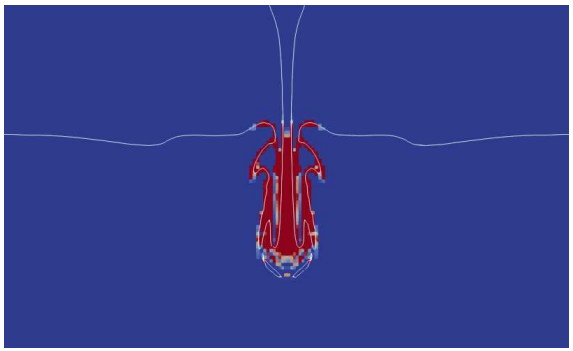
(a) `interAirEntFoam` (b) `interFoam`

Figure: Vertical plunging jet, 2D

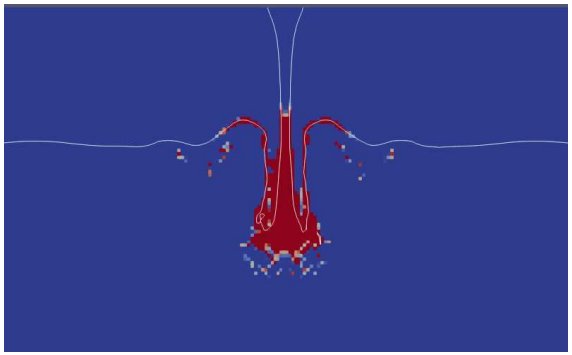
Vertical plunging jet – results



(a) t=0.2 sec



(b) t=0.5 sec



(c) t=0.8 sec

Figure: Indication of where the source term is active